SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

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U.S. Environmental Protection Agency
Office of Superfund Remediation and Technology Innovation
1200 Pennsylvania Avenue, NW (5204P)
Washington, DC 20460

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ACRONYMS and ABBREVIATIONS

AALAC Ambient Aquatic Life Advisory Concentrations

ACGIH American Conference of Governmental Industrial Hygienists

ATSDR Agency for Toxic Substances and Disease Registry

AWQC Ambient Water Quality Criteria

BCF Bioconcentration Factor

CAS RN Chemical Abstracts Survey Registration Number

CCC Criteria Continuous Concentration

CERCLA Comprehensive Environmental Response, Compensation, and Liability Act

CFR Code of Federal Regulations
CMC Criteria Maximum Concentration

ED Effective Dose

EPA United States Environmental Protection Agency

EPI Estimation Programs Interface

FDAAL Food and Drug Administration Action Levels

f_S Sorbent Content (fraction of clays plus organic carbon)

HEAST Health Effects Assessment Summary Tables
HEDR Handbook of Environmental Degradation Rates

HLC Henry's Law Constant HRS Hazard Ranking System HTF Human Toxicity Factor

ICRP International Commission on Radiological Protection

Int Intermediate

IRIS Integrated Risk Information System

IUR Inhalation Unit Risk

K_d Soil/Water Distribution Coefficient

Koc Soil Organic/Carbon Partition Coefficient

LC Lethal Concentration

LD Lethal Dose

Log K_{OW} Logarithm of the n-Octanol-Water Partition Coefficient

MCI Molecular Connectivity Index
MCLs Maximum Contaminant Levels
MCLGs Maximum Contaminant Level Goals

MRL Minimal Risk Level MW Molecular Weight

NAAQS National Ambient Air Quality Standards

NESHAPs National Emission Standards for Hazardous Air Pollutants

NHL Non-Hodgkin's Lymphoma

NIOSH National Institute for Occupational Safety and Health NJDEP New Jersey Department of Environmental Protection

NPL National Priorities List

OEHHA California Environmental Protection Agency Office of Environmental Health Hazard

Assessment

OSRTI Office of Superfund Remediation and Technology Innovation

PAH Polyaromatic Hydrocarbons PCB Polychlorinated Biphenyls

PPRTV Provisional Peer Reviewed Toxicity Values

PRG Preliminary Remediation Goals
RBA Relative Bioavailability Adjustment

REL Reference Exposure Level RfC Reference Concentration

RfD Reference Dose

RME Reasonable Maximum Exposure

RTECS Registry of Toxic Effects of Chemical Substances

RTI Research Triangle Institute SC Screening Concentration

SCDM Superfund Chemical Data Matrix

SF Slope Factor (Cancer)

SPHEM Superfund Public Health Evaluation Manual

SRC Syracuse Research Corporation

STSC Superfund Health Risk Technical Support Center

TCDD 2,3,7,8-Tetrachlorodibenzo-p-dioxin

TCE trichloroethylene

TEF Toxicity Equivalence Factor

UMTRCA Uranium Mill Tailings Radiation Control Act

WOE Weight-of-Evidence

SUPERFUND CHEMICAL DATA MATRIX (SCDM) METHODOLOGY

[June 2014]

1.0 INTRODUCTION

The Superfund Chemical Data Matrix (SCDM) contains factor values and screening concentration benchmarks that can be used when applying the Hazard Ranking System (HRS; 40 CFR Part 300 Appendix A, 55 FR 51583) to evaluate potential National Priorities List (NPL) sites. The HRS assigns factor values for toxicity, gas migration potential, gas and ground water mobility, surface water persistence, and bioaccumulation potential. These assignments are based on the physical, chemical, ecological, toxicological, and radiological properties of hazardous substances present at a site. Hazardous substances, as defined for HRS purposes, include both hazardous substances referenced in the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) section 101(14), which are substances specifically listed under other federal laws and are known as "CERCLA hazardous substances," and "pollutants or contaminants" as defined in CERCLA itself in section 101(33).

SCDM contains HRS factor values and benchmarks for those hazardous substances frequently found at sites that are evaluated using the HRS. SCDM also contains the physical, chemical, toxicological, and radiological input data used to calculate the factors and benchmarks. The input data presented in SCDM are taken directly from peer reviewed, generally accepted literature sources and databases and/or U.S. Environmental Protection Agency (EPA) developed literature sources and databases; or are calculated using procedures set forth by the EPA and in the HRS. Further HRS procedures are then applied to the input data to determine factor values and benchmarks, which include both risk-based screening concentrations and concentrations specified in regulatory limits for the hazardous substances.

This document explains the procedures used to provide chemical and physical properties, factor values and screening concentration benchmarks for substances listed in SCDM. The factor values and benchmarks supersede any previous values provided by SCDM, beginning January 2014. These new values and benchmarks reflect the EPA's methodology for determining risk, as described in the EPA's Risk Assessment Guidance for Superfund (RAGS) Volume 1: Human Health Evaluation Manual, Part F: Supplemental Guidance for Inhalation Risk Assessment and Part B: Development of Risk-based Preliminary Remediation Goals (EPA-540-R-070-002/OSWER 9285.7-82) and Soil Screening Guidance: Technical Background Document (EPA/540/R95/128).

Section 2.0 (Data Selection Methodology) of this document explains how data are selected and prioritized for use in assigning SCDM values. Section 3.0 (Calculation of Interim Values) describes how some values (e.g., half-lives, distribution coefficients, slope factors and water solubility for metals) are calculated using data and methodologies from published literature or regulatory guidance documents. Section 4.0 (Screening Concentration Benchmarks) describes how screening concentration benchmarks are calculated for air, water, soil and human food chain exposures. Section 5.0 (SCDM Data Reporting and Appendices) describes how SCDM data, HRS factor values, and screening concentration benchmarks are presented in the SCDM Appendices.

Data inputs, factor values and benchmarks are listed, by substance, in SCDM Appendix A. Appendices BI and BII contain tables presenting HRS factor values and benchmarks, organized by pathway. Appendix C contains a cross-reference index of substance name synonyms.

2.0 DATA SELECTION METHODOLOGY

This section describes the methodology used for collecting and selecting data to determine factor values and screening concentration benchmarks for the substances listed in SCDM. It also specifies data source reference hierarchies and how the hierarchies are applied for each data type.

Section 2.1 describes hazardous substance identification protocols and how they relate to special cases. Sections 2.2 through 2.9 specify the references used to obtain data and the methodologies used to extract the data and assign values. The criteria described in these sections were developed based on the type and quality of data available in the current SCDM references; they are not intended to apply to all data in general.

2.1 General Protocols for SCDM Data Collection

Compiling data for SCDM requires a determination of which data reasonably apply to each hazardous substance. In most cases, data are collected for each substance from the specific references identified in Sections 2.2 through 2.8. In some cases, however, data in the references cited are available only for a class or mixture of hazardous substances and not for the individual substances that are included in the class or that make up the mixture. In general, if any of these classes or mixtures is present at a hazardous waste site, it is assumed that the most toxic, most persistent, or most bioaccumulative component of the class or mixture is present. For these mixtures or classes, SCDM collects and uses those data resulting in the greatest HRS factor values as specified by the HRS (e.g., lowest Reference Dose [RfD], highest cancer slope factor [SF], longest half-life and greatest bioaccumulation factor) from the data provided in the references used. In other cases, data that are specific to individual substances are used or substituted as representative for a class of substances. These special cases are described in Sections 2.1.1 through 2.1.4 below.

2.1.1 Generic Values

SCDM contains generic values for the following classes of compounds:

- Chromium (III and VI oxidation states) SCDM contains values for chromium III, chromium VI, and a "generic" total chromium value to be used only when the specific oxidation state is not known. SCDM assigns the oral RfD and reference concentration (RfC) from chromium VI to total chromium.
- Mercury (elemental and inorganic compounds) SCDM contains data for elemental and inorganic
 species of mercury, and applies the data to a single listing of "mercury." The oral RfD is for mercuric
 chloride, and the inhalation RfD is for elemental mercury vapor. The vapor pressure, Henry's Law
 Constant and distribution coefficient are for elemental mercury. A geometric mean water solubility is
 based on the lowest solubility (mercurous chloride) and highest solubility (mercury perchlorate) found
 in the reference sources.
- Polychlorinated biphenyls (PCBs) PCBs are represented as a single class of compounds, regardless of
 the PCB mixture or mixtures that may be identified at a site. For PCBs, toxicity in SCDM is based on
 Arochlor 1254, which results in the most environmentally conservative screening concentration
 benchmarks and bioaccumulation/human food chain-based factor values for this group of compounds.
 EPA's most recent reference on PCB risk assessment is "EPA's PCB Risk Assessment Review Guidance
 Document, Interim Draft," 2000a.

• Endosulfans – SCDM contains data for endosulfan mixture and two endosulfan isomers (endosulfan I and endosulfan II). The RfD and distribution coefficient data are collected for endosulfan and applied to endosulfan mixture and its isomers. SCDM contains a vapor pressure and Henry's Law constant for each isomer.

• Chlordane (alpha and gamma) – SCDM contains some data for the alpha and gamma isomers of chlordane, but most values represent a mixture of the two. When a reference does not specify whether chlordane data were derived from a specific isomer or isomer concentration, SCDM uses the generic values.

2.1.2 Use of Compound Classes to Assign Values for Individual Substances

SCDM assigns substance class data to the substances listed below. If no data can be found in the specified references for an individual substance, but data are available for the generic class to which the substance belongs, SCDM assigns the generic value to that substance. These substance classes contain relatively small sets of isomers, which are likely to occur as mixtures, and are well defined, in that the generic class typically refers to a mixture of all members of the class (e.g., o-, m-, p-xylenes). Members of these classes are also expected to have similar chemical behavior.

- Polychlorinated dibenzo-dioxins and furans SCDM contains cancer slope factor, inhalation unit risk (IUR) and RfD values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). When a slope factor, IUR and/or RfD are not available for similar dioxins and furans listed in SCDM, SCDM applies toxicity equivalence factors (TEFs) to determine the values for these substances. Substance-specific TEFs are obtained from EPA's Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and Dioxin-Like Compounds (EPA/100/R 10/005), December 2010. All members of this class are assigned the weight of evidence (WOE) assigned to TCDD, which is currently B2.
- Polyaromatic hydrocarbons (PAHs) SCDM contains cancer slope factor and IUR values for benzo(a)pyrene. When a slope factor and/or IUR are not available for similar PAHs listed in SCDM, SCDM applies TEFs to determine values for these substances. PAH-specific TEFs are obtained from EPA's Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089), July 1993.
- Xylenes Values are provided for o-xylene, m-xylene and p-xylene. If no data can be found in the specified references for the individual substances, but data are available for the generic class of xylenes, SCDM assigns the generic value to the individual substances. The class of xylenes is a relatively small set of isomers that are likely to occur as mixtures. The class also is well defined in that the generic class (e.g., xylenes) almost always refers to a mixture of all members of the class (o-, m-, and p-xylene). The expected similarity in chemical behavior for members of each class, as well as the likelihood that they will occur as mixtures, makes using data from mixtures reasonable.
- Dibutyltin compounds SCDM assigns an RfD for dibutyltin dichloride using the following molecular weight conversion of the RfD assigned to dibutyltin: RfD (dibutyltin dichloride) = RfD (dibutyltin) x [molecular weight (dibutyltin dichloride) / molecular weight (dibutyltin)].
- Tributyltin compounds SCDM assigns an RfD for tributyltin chloride using the following molecular weight conversion of the RfD assigned to tributyltin: RfD (tributyltin chloride) = RfD (tributyltin) x [molecular weight (tributyltin chloride) / molecular weight (tributyltin)].

2.1.3 Substitution Classes

In some cases, SCDM uses data from a parent substance class, for particular substances of that class. SCDM contains three major classes of data for which data substitution may be applied: (1) toxicity, (2) ground water mobility and (3) other. All toxicity data used to determine human- or eco-toxicity factor values can be substituted. Ground water mobility data substitutions include water solubility, geometric mean water solubility and soil/water distribution coefficient (K_d). Parent class data also may be used for hydrolysis, biodegradation, photolysis and volatilization half-lives, as well as bioconcentration factor (BCF) and logarithm of the n-octanol-water partition coefficient (Log K_{OW}).

Currently in SCDM, two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for ground water mobility values with the elemental metal as the class parent. Radioactive isotopes may inherit data from the primary radioactive element. Substitute data are not applied to radioactive isotope decay chains.

2.1.4 Substances with Unique Value Selection

- Cadmium For cadmium, the Integrated Risk Information System (IRIS) contains two RfD values: one for
 drinking water and one for dietary exposure. Because SCDM calculates RfD-based, non-cancer screening
 concentration benchmarks for both drinking water and dietary exposures, the more conservative value is
 used; therefore, SCDM uses the drinking water RfD for cadmium.
- Asbestos and Lead The HRS specifies that a human toxicity factor of 10,000 be assigned to asbestos, lead
 and lead compounds. Asbestos also receives a K_d value of 1,000, as stated in the HRS.
- Copper SCDM uses a HEAST water quality standard of 1.3 mg/L to determine an RfD for copper, based on drinking water exposure assumptions of 70 kg body mass, 30 years exposure, and 1L/day ingestion.
- Vanadium SCDM assigns an RfD that has been identified for vanadium pentoxide as the RfD for vanadium.

2.2 Data Used to Determine Human Toxicity Factor Values and Screening Concentration Benchmarks

Section 2.2 details how data are obtained for determining human toxicity factor (HTF) values and screening concentration benchmarks. RfD, RfC, SF, IUR, lethal dose with 50% mortality (LD_{50}), lethal concentration with 50% mortality (LC_{50}) and effective dose (ED_{10}) values are identified and used to determine the HTF value for each substance according to HRS Section 2.4.1.1. The RfD, RfC, SF, IUR values are also used to determine screening concentration benchmarks (see Section 4.0 of this document).

Non-carcinogenic data (RfD, RfC, LD_{50} and LC_{50}) and carcinogenic data (IUR, SF and ED_{10}) are selected for each substance according to a hierarchy of references. Of the values selected, the most conservative (i.e., most protective of human health) is used to determine the HTF, regardless of exposure route or whether the value represents a non-cancer or cancer effect.

2.2.1 SF, IUR, RfD and RfC Data Collection

SCDM does not assign RfD or RfC data to radionuclides. SF values (inhalation, oral and external exposure) are obtained for radionuclides from the following references, listed in order of preference:

- U.S. EPA *Preliminary Remediation Goals (PRGs) for Radionuclides*. Office of Superfund Remediation and Technology Innovation (OSRTI). http://epa-prgs.ornl.gov/radionuclides/download.html. Accessed October 2012.
- U.S. EPA. Health Effects Assessment Summary Tables (HEAST). Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/. Accessed September 2012.

For all other substances, RfD and RfC values are obtained from the following references, listed in order of preference:

- U.S. EPA. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris. Accessed October 2012.
- Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs) derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. http://hhpprtv.ornl.gov. Accessed September 2012.
- The Agency for Toxic Substances and Disease Registry (<u>ATSDR</u>) minimal risk levels (<u>MRLs</u>). http://www.atsdr.cdc.gov/mrls/mrllist.asp (non-cancer data only) Accessed September 2012.
- The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp. Accessed September 2012.
- PPRTV Appendix, http://hhpprtv.ornl.gov/quickview/pprtv compare.php. Accessed September 2012.
- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/. Accessed September 2012.

ATSDR provides MRLs for acute (1 – 14 days), intermediate (>14 – 364 days), and chronic (365 days and longer) exposure durations. During SCDM data collection, preference is given to ATSDR values that are based on chronic exposure. Where chronic exposure values are not available, SCDM uses values based on intermediate exposure. Where intermediate MRLs are used in SCDM, the reference provided in the SCDM Appendices is "ATSDR-Int." SCDM does not use MRLs that are based on acute exposure.

For non-radionuclide substances, SF and IUR values are obtained from the following references, listed in order of preference:

• U.S. EPA. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris. Accessed October 2012.

 Provisional Peer Reviewed Toxicity Values for Superfund (PPRTVs) derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. http://hhpprtv.ornl.gov. Accessed September 2012.

- The California Environmental Protection Agency (CALEPA) Office of Environmental Health Hazard Assessment's (OEHHA) Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp. Accessed September 2012.
- PPRTV Appendix. http://hhpprtv.ornl.gov/quickview/pprtv compare.php. Accessed September 2012.
- U.S. EPA. Health Effects Assessment Summary Tables (HEAST). Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/. Accessed September 2012.

An oral cancer slope factor was not available for chromium VI, from the first three references listed (IRIS, PPRTV, ATSDR); an oral cancer slope factor from the New Jersey Department of Environmental Protection (NJDEP Division of Science, Research and Technology, *Derivation of Ingestion-Based Soil Remediation Criterion for Cr+6 Based on the NTP Chronic Bioassay Data for Sodium Dichromate Dihydrate*, April 2009. http://www.state.nj.us/dep/dsr/chromium/soil-cleanup-derivation.pdf) includes consideration of mutagenicity, and was preferred over the slope factor provided in CALEPA OEHHA.

2.2.2 Weight of Evidence (WOE)

When available, a carcinogenic risk WOE classification is collected from the same reference that provided the corresponding cancer risk value (e.g., IUR or SF). If only an oral WOE classification is provided for a substance that is identified as carcinogenic via inhalation, the oral WOE is recorded for the inhalation cancer risk value. In some instances, two or more WOE assessments are provided in a single reference. In these cases, the WOE assessment associated with the selected risk value is used; typically, this is the most recent WOE assessment.

2.2.3 LD_{50} – Oral, Dermal; LC_{50} - Inhalation

When no RfD, RfC, cancer SF with WOE or IUR with WOE are available, SCDM uses an LD_{50} (oral, dermal) or LC_{50} (dust and gas inhalation) to assign HTF values. The lowest value is used to determine the HTF. LD_{50} and LC_{50} values are not used to calculate screening concentration benchmarks.

SCDM does not assign LD_{50} and LC_{50} values to radionuclides. The references used to collect these data for other substances are listed below, in order of preference:

- American Conference of Governmental Industrial Hygienists (ACGIH). 2012. Threshold Limit Values and Biological Exposure Indices, ACGIH, Cincinnati, OH.ISBN: 978-1-607260-48-6. http://www.acgih.org/store/ProductDetail.cfm?id=2190.
- National Institute for Occupational Safety and Health (NIOSH). 2012. Registry of Toxic Effects of Chemical Substances (RTECS). http://www.cdc.gov/niosh/rtecs/.

SCDM contains the lowest LD_{50} or LC_{50} value for any mammalian species by the oral and dermal exposures, in controlled dose studies, with durations of less than 24 hours. LD_{50} and LC_{50} data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.

2.2.4 ED₁₀ and Weight-of-Evidence – Oral, Inhalation

When a cancer SF with WOE is not available, SCDM uses ED_{10} oral and inhalation values to calculate cancer SF (see Section 3.3 of this methodology document). SCDM does not assign ED_{10} values to radionuclides. For all other substances, SCDM uses data from the following references, listed in order of preference for oral and inhalation ED_{10} and associated WOEs:

- U.S. EPA. 1989. *Methodology for Evaluating Potential Carcinogenicity in Support of Reportable Quantity Adjustments Pursuant to CERCLA Section 102* (EPA_ED10), Office of Health and Environmental Assessment, Washington DC (EPA/600/8-89/053).
- U.S. EPA. 1986. *Superfund Public Health Evaluation Manual* (SPHEM), Office of Emergency and Remedial Response, Washington DC (EPA/540/1-86/060) (OSWER Directive 9285, 4-1).

 ED_{10} data that are reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.

2.3 Mobility Information

Vapor pressures and Henry's Law Constants are used to determine the gas migration potential and gas mobility potential for each substance. Water solubility and soil/water distribution coefficients are used to determine ground water mobility factor values. Henry's Law Constants are also used to determine volatilization half life.

2.3.1 Vapor Pressure

SCDM uses data from the following references to obtain vapor pressures for organic compounds, listed in order of preference:

- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- The Estimation Programs Interface (EPI) SuiteTM (experimental values). Developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed September 2012.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- CRC Handbook of Chemistry and Physics, 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

SCDM uses data from the following references to obtain vapor pressures for non-organic compounds, listed in order of preference:

- CRC Handbook of Chemistry and Physics, 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

If a recommended vapor pressure is not provided in the references, SCDM uses a value measured at 25°C. If more than one vapor pressure measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If no temperature is specified for all vapor pressure measurements for a substance, SCDM uses the highest value.

If no vapor pressure values are available in any of the references listed or if the referenced value is suspect, a value may be either selected from a data source outside the hierarchy or estimated. For any given substance, suspect values are identified by comparison with other vapor pressure values in SCDM data sources or other sources of chemical property data. The procedures described in Lyman *et al.* (1990) are used to estimate vapor pressure. RTI (1996) describes the use of these procedures for specific hazardous substances.

 Estimation procedures set forth by Lyman *et al.* 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996.
 Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

For organic substances, if a vapor pressure is not available, a normal boiling point is obtained from the reference hierarchy listed in Section 2.8.1. If the boiling point at 1 atmosphere (atm) is <25°C, a default vapor pressure of 760 Torr is used with the assumption that the substance is a gas at 25°C.

If no vapor pressure is available for a substance and the normal boiling point is \geq 25°C, SCDM assumes that the substance is in a particulate form, rather than a gaseous form, and no vapor pressure is assigned. This assumption is made because the absence of a vapor pressure value often reflects an extremely low and difficult to measure (under standard conditions) value for nongaseous substances.

2.3.2 Henry's Law Constant

SCDM uses data from the following references to obtain Henry's Law Constants (HLC) for organic compounds, listed in order of preference:

• PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.

 EPI SuiteTM (experimental values). Developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed September 2012.

• CHEMFATE Database. Syracuse Research Corporation (SRC). Syracuse, NY http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381. Accessed December 2012.

SCDM uses data from the following references to obtain HLC's for inorganic compounds, listed in order of preference:

- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all Henry's Law Constants for a substance, SCDM uses the highest value.

2.3.3 Water Solubility

Water solubility is used, along with K_d values, to calculate the ground water mobility of hazardous substances that do not meet observed release criteria. All hazardous substances that are available to migrate from sources at a site to the ground water are evaluated for ground water mobility. Water solubility values are also used to assign BCF values for hazardous substances when BCF or Log K_{OW} data are not available.

2.3.3.1 Water Solubility - Organic Substances

SCDM obtains water solubility values for organic substances from the following references, listed in order of preference:

- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- EPI SuiteTM (experimental values) developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC).
 http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April November 2012.

CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Estimation procedures set forth by Lyman et al. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all water solubility measurements for a substance, SCDM uses the highest value.

2.3.3.2 Water Solubility – Metals, Metalloids and Radionuclides

SCDM obtains water solubility values for metals and metalloid compounds from the following references, listed in order of preference:

- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

For a metal or metalloid substance, SCDM determines and assigns water solubility as the geometric mean of the highest and lowest water solubility values available for compounds containing the metal or metalloid, as defined in the HRS (see HRS Section 3.2.1.2, Mobility) and described in Section 3.7 of this document.

2.3.4 Soil/Water Distribution Coefficient (Kd); Soil Organic/Carbon Partition Coefficients (Koc and Log Kow)

 K_d values are used to calculate ground water mobility for hazardous substances that do not meet observed release criteria. If K_d values are not available, associated K_{oc} and $Log\ K_{ow}$ values are used to calculate K_d . All

hazardous substances that are available to migrate from sources at the site to ground water are evaluated for ground water mobility.

For organic substances, SCDM calculates the K_d according to HRS Section 3.2.1.2 (Mobility) and the relationship of $K_d = K_{OC} \times f_S$ (see Section 3.6 of this methodology document), where f_S is the sorbent content (fraction of clays plus organic carbon) and K_{OC} is obtained from the following references, listed in order of preference:

- EPI SuiteTM (estimated values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April - November 2012.
- U.S. EPA. 2002. Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (Peer Review Draft), OSWER 9355.4-24. http://www.epa.gov/superfund/health/conmedia/soil/pdfs/ssg_main.pdf. Accessed August 2012.
- EPI SuiteTM (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. April - November 2012
- Estimated as described in Section 3.6 of this methodology document

When using values from EPI SuiteTM, SCDM prefers K_{OC} values that are estimated using the Molecular Connectivity Index (MCI) method over K_{OC} values that are estimated by the Log K_{OW} method. When a K_{OC} is not available using the MCI method, SCDM uses the EPI SuiteTM K_{OC} values estimated using the Log K_{OW} method. Information regarding collection of Log K_{OW} values is provided in Section 2.5.2 of this methodology document. Section 3.6 (Soil Water Distribution Coefficient [Kd]; Soil Organic/Carbon Partition Coefficients [Koc]) of this document provides additional information regarding SCDM calculations of Kd and K_{OC} values.

SCDM obtains K_d values for inorganic substances from the following references, listed in order of preference:

- U.S. EPA. 2002. Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (Peer Review Draft), Office of Solid Waste and Emergency Response. 9355.4-24. http://www.epa.gov/superfund/health/conmedia/soil/pdfs/ssg_main.pdf. Accessed August 2012.
- U.S. EPA. 1996. Soil Screening Guidance: Technical Background Document. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502. http://www.epa.gov/superfund/health/conmedia/soil/index.htm. Accessed August 2012.
- Baes, C.F. III, R.D. Sharp, and A.L. Sjoreen, and R.W. Shor. 1984. A Review and Analysis of Parameters for Assessing Transportation of Environmentally Released Radionuclides through Agriculture. Oak Ridge National Laboratory, TN. ORNL-5786.
- HRS Section 3.2.1.2 (See Section 3.6 of this methodology document).

SCDM contains values corresponding to typical subsurface pH (e.g., 6.8).

2.4 Persistence Information

The evaluation of persistence is based primarily on the half-life of hazardous substances in surface water and (for non-radionuclides) secondarily on the sorption of the hazardous substances to sediments. Persistence information is used to determine the surface water persistence factor value.

2.4.1 Hydrolysis, Biodegradation and Photolysis Half-Lives

SCDM does not assign hydrolysis, biodegradation or photolysis half lives to radionuclides. SCDM obtains hydrolysis, biodegradation and photolysis half-lives for all other substances from the following references, listed in order of preference:

- CHEMFATE Database. SRC. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381. Accessed December 2012.
- *Handbook of Environmental Degradation Rates* (HEDR). 1991. Howard, Phillip H., W.F. Jarvis, W.M. Meylan and E.M. Michalenko, Lewis Publishers, Inc. Chelsea, Michigan.

SCDM only uses values that have been measured in water from the CHEMFATE database. SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, a value determined at a temperature closest to 25°C is selected. If no temperature is specified for all half-life values for a substance, SCDM uses the highest value. If values are obtained from HEDR, SCDM uses only values listed as "first-order." If multiple values are provided, the highest value is used.

2.4.2 Volatilization Half-Lives

SCDM estimates volatilization half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.4 of this methodology document. Volatilization half-lives are not collected or estimated for inorganic substances.

2.4.3 Radioactive Half-Lives

SCDM obtains radioactive half-lives for radioactive substances from the following references, listed in order of preference:

- U.S. EPA. *Health Effects Assessment Summary Tables (HEAST)*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/. Accessed September 2012.
- U.S. EPA. October 2000. *Soil Screening Guidance for Radionuclides: User's Guide*. EPA/540-R-00-007 PB2000 963307. http://www.epa.gov/superfund/health/contaminants/radiation/radssg.htm. Accessed August 2012.

2.5 Bioaccumulation Potential Information

BCF values for freshwater and saltwater (one set each for the human food chain and environmental threats) are used to determine bioaccumulation potential factor values (40 CFR Part 300, Appendix A, Section 4.1.3.2.1.3). BCF values are selected based on edible species to determine bioaccumulation potential factor values for the human food chain threat. If BCF data are not available for organic substances, the Log K_{OW} is used to determine

bioaccumulation potential factor values. Water solubility data are used if the Log K_{OW} exceeds 6.0, the substance is inorganic or there is no Log K_{OW} .

2.5.1 Bioconcentration

Bioaccumulation factor values in SCDM are preferentially based on actual measurements of bioconcentration in aquatic organisms. SCDM used BCF values from the following sources, listed in order of preference:

- U.S. EPA. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/ecotox. Accessed September 2012.
- Versar, Inc. 1990. *Issue Paper: Bioaccumulation Potential Based on Ambient Water Quality Criteria Documents* (VER_BCF). Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC. Contract No. 68-W8-0098.

SCDM uses the highest measured value from ECOTOX. Measured values are preferred over calculated or estimated values. The Versar reference is a report of literature survey BCF values developed to obtain preliminary values for use when the initial HRS was being developed. When using data from this reference, SCDM also prefers the highest measured value to an estimated value. BCF data reported in the references as less than or greater than a particular value are considered non definitive and are not used in SCDM.

<u>Environmental Threat:</u> For the environmental threat, the highest value from any aquatic organism, regardless of whether it is consumed by humans, in each reference is used to establish environmental threat BCF values.

<u>Human Food Chain Threat:</u> The highest measured BCF for aquatic organisms typically known to be consumed by humans is used to obtain the human food chain threat BCF values. Table 1 includes a list of some of the organisms for which these BCF values may be taken. This list is intended to serve only as a guide to the SCDM data collector and hence, not all human food chain aquatic organisms are listed. Values from organisms not in this list may be used provided they are known to be consumed by humans.

Table 1. Examples of Human Food Chain Aquatic Organisms

American or Virginia	Carp	Kiyi	Red abalone
oyster	Chinook salmon	Lake trout (siscowet)	Red swamp crayfish
Asiatic clam	Channel catfish	Lake whitefish	River salmon
Atlantic dogwinkle	Clam	Largemouth bass	Rock bass
Atlantic salmon	Cockle	Limpet	Rough periwinkle
Atlantic silverside	Coho salmon	Lobster	Sauger
Bay scallop	Common bay mussel	Mangrove snapper	Scallop
Bent-nosed clam	Common mirror colored	Marsh snail	Shrimp
Bivalve/clam/mussel	Carp	Mussel	Sole
Black abolone	Common shrimp	Netted dog whelk	Spot
Black bullhead	Crab	Northern anchovy	Striped bass
Black crappie	Crayfish	Northern krill	Striped mullet
Black mussel	Dungeness or edible crab	Northern pike	Swan mussel
Blue crab	Eel	Oyster	Taiwan abalone
Bluegill	Filefish	Pilchard sardine	Tong sole
Bony fishes	Flounder	Pinfish	Topmouth gudgeon (golden shiner)
Brook silverside	Giant gourami	Pink salmon	White mullet
Brook trout	Green sunfish	Porgy	White sand mussel

Brown trout	Golden shiner	Prawn	Whiting
Brown shrimp	Gudgeon	Rainbow trout	Winkle, common edible
Bull frog	Gulf toadfish		

2.5.2 Octanol/Water Partition Coefficient (Log Kow)

Log K_{OW} values are used to determine the bioaccumulation potential factor value for a hazardous substance for which BCF data are not available. SCDM may also use the log K_{OW} to estimate a log K_{OC} when a K_{OC} is not available (see Sections 2.3.4 and 3.2 of this methodology document). SCDM obtains n-octanol/water (log K_{OW} , also referred to as Log P) values from the following sources, listed in order of preference:

- EPI SuiteTM (organic substances, experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April November 2012.
- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- CHEMFATE Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381. Accessed December 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development. Prepared for the U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

SCDM uses experimental values; estimated or calculated values are not used. If values are obtained from CHEMFATE, the recommended values are used.

2.5.3 Water Solubility

Water solubility values are used to assign a bioaccumulation potential factor value for hazardous substances when BCF or log K_{OW} data are not available. See Sections 2.3.3.1 (Water Solubility – Organic Substances) and 2.3.3.2 (Water Solubility – Metals, Metalloids and Radionuclides) of this methodology document for the data collection protocol and guidance on water solubility values.

2.6 Ecotoxicity Parameters

Ecotoxicity data are used in the HRS scoring system to determine the Ecotoxicity Factor values (HRS; 40 CFR Part 300, Appendix A, Section 4.1.4.2.1.1). SCDM uses acute and chronic freshwater and saltwater criteria, and only uses those values specifically stated as criteria. If criteria are not available, then LC_{50} data are used.

2.6.1 Acute and Chronic Freshwater and Saltwater Criteria - CCC, CMC

The HRS (Section 4.1.4.2.1.1, Ecosystem Toxicity) uses the EPA Ambient Water Quality Criteria (AWQC) and Ambient Aquatic Life Advisory Concentrations (AALAC) for assigning ecosystem toxicity factor values. The

acute and chronic AWQC have been replaced by a new set of criteria, and the AALAC values no longer exist. The new criteria replacing the AWQC for both freshwater and saltwater are labeled as (1) Criteria Maximum Concentration (CMC), to be used in place of what was previously acute AWQC, and (2) Criteria Continuous Concentration (CCC), to be used in place of what was previously chronic AWQC. These new values closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been rederived using different methodology. Therefore, the resulting values must be used as directed by the EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. Some CMC and CCC values are baseline values that must be adjusted using the information specified in the endnotes. The CMC and CCC values are taken from:

 U.S. EPA. National Recommended Water Quality Criteria. Office of Water. Washington, DC. http://water.epa.gov/scitech/swguidance/standards/current/index.cfm#altable. Accessed October 2012.

2.6.2 LC50 - Freshwater, Saltwater

SCDM obtains LC₅₀ data from the ECOTOX database for both freshwater and saltwater.

• U.S. EPA. 2012. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/ecotox. Accessed September 2012.

SCDM uses the lowest acute LC_{50} value found for any aquatic organism in the specified environment with an acute exposure duration of ≥ 1 day and ≤ 4 days. When no duration or environment is given, LC_{50} values are not entered into SCDM.

2.7 Regulatory Benchmarks

The HRS assigns extra weight to targets with exposure to hazardous substances at levels that are at or above regulatory benchmark values. This section describes the sources for regulatory limits that the HRS uses as health-based or ecological-based benchmarks.

2.7.1 National Ambient Air Quality Standards (NAAQS)

National Ambient Air Quality Standards (NAAQS) are used to establish Level I concentrations. Targets exposed to concentrations at or above the NAAQS are scored as Level I targets. SCDM uses data from the following source to obtain NAAQS:

• 40 CFR Part 50. National Ambient Air Quality Standards. http://www.epa.gov/air/criteria.html. Accessed October 2012.

2.7.2 National Emissions Standards for Hazardous Air Pollutants (NESHAPs)

National Emission Standards for Hazardous Air Pollutants (NESHAPs) are used to establish Level I concentrations. Targets exposed to concentrations at or above NESHAPs are scored as Level I targets. SCDM uses data from the following source to obtain NESHAPs and uses only those values that are reported in ambient concentration units (μ g/m³):

• 40 CFR Part 61 and Part 63. National Emission Standards for Hazardous Air Pollutants. http://www.epa.gov/compliance/monitoring/programs/caa/neshaps.html. Accessed October 2012.

2.7.3 Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs)

Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs) are used to establish Level I concentrations. Targets exposed to concentrations at or above MCLs and MCLGs are scored as Level I targets. SCDM uses data from the following sources for MCLs and MCLGs:

- U.S. EPA. 2009. National Primary Drinking Water Standards. Accessed through List of Drinking Water Contaminants and MCLs. Office of Water, Washington, DC. http://water.epa.gov/drink/contaminants/index.cfm. Accessed October 2012.
- U.S. EPA. October 2000. *Soil Screening Guidance for Radionuclides: User's Guide* (EPA/540-R-00-007, PB2000 963307). http://www.epa.gov/superfund/health/contaminants/radiation/radssg.htm. Accessed August 2012.

SCDM uses only MCLs that are reported in units of concentration (mg/L, μ g/L or pCi/L) and only non-zero MCLGs that are reported in units of concentration (mg/L or μ /L). For substances where multiple values are listed, SCDM uses the lowest value. For substances where both MCLs and MCLGs are provided but are different, SCDM selects the lower of the two values.

2.7.4 FDA Action Levels (FDAALs)

Food and Drug Administration Action Levels (FDAAL) are used to establish Level I concentrations. Targets exposed to concentrations at or above FDAALs are scored as Level I targets. SCDM contains FDAALs for fish and shellfish only, and obtains the FDAAL values from the following reference:

 U.S. Food and Drug Administration. 2000. Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed. Center for Food Safety and Applied Nutrition, Washington, D.C. http://www.fda.gov/Food/GuidanceComplianceRegulatoryInformation/GuidanceDocuments/ChemicalContaminantsandPesticides/ucm077969.htm. Accessed October 2012.

2.7.5 Ecological Based Benchmarks

See Section 2.6.1 of this document for information regarding acute CMC and chronic CCC for freshwater and saltwater.

2.7.6 Uranium Mill Tailings Radiation Control Act Standards (UMTRCA)

Uranium Mill Tailings Radiation Control Act (UMTRCA) standards are used to establish Level I concentrations. Targets exposed to concentrations at or above UMTRCA standards are scored as Level I targets. SCDM extracts UMTRCA data directly from 40 CFR Part 192 (Uranium Mill Tailings Radiation Control Act Standards). http://www.wise-uranium.org/ulus.html. Accessed October 2012.

2.8 Physical Properties

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point and melting point. SCDM applies yes/no flags to classify physical property data into the four substance categories defined below.

Organic Substances ("Organic"): "Y" indicates that the substance is organic, and "N" indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential. Volatile and semivolatile organics are indicated. These flags influence the SCDM calculation of K_d values.

Metal-Containing Substances ("Metal Contain"): "Y" indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. "N" indicates that the substance is not, or does not contain, a metal or metalloid. This flag is used to determine factor values for ground water mobility and surface water persistence.

Radioactive Isotope ("**Radionuclide**"): "Y" indicates that the substance is a specific radioactive isotope, and "N" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag is used to determine factor values for human toxicity, ecosystem toxicity and surface water persistence.

Radioactive Element ("Rad. Element"): "Y" indicates that the substance is a radioactive element, and "N" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag determines whether or not the HRS factors and benchmarks are printed in Appendix A.

2.8.1 Chemical Formula, Boiling Point and Melting Point

Chemical formula, boiling point and melting point data are extracted for inorganic substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Chemical formula, boiling point and melting point data are extracted for all other substances, from the following sources in order of preference:

- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

• EPI SuiteTM (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April - November 2012.

Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

2.8.2 Molecular Weight

Molecular weight data are collected for inorganic substances, from the following sources in order of preference:

- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Molecular weight data are collected for all other substances, from the following sources in order of preference:

- EPI SuiteTM (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC).
 http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April - November 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

2.8.3 *Density*

Density data are collected for inorganic substances, from the following sources in order of preference:

 CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 – 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

• PHYSPROP Database. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed September 2012.

- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008. Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- O'Neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

Density data are collected for all other substances, from the following sources in order of preference:

- EPI SuiteTM (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed April November 2012.
- CRC Handbook of Chemistry and Physics. 93rd Edition. 2012 2013. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Lange's Handbook of Chemistry. 16th Edition. 2004. Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

3.0 CALCULATION OF INTERIM VALUES

SCDM calculates specific chemical properties for some of the following cases:

- when all preferred references do not contain a property value for a given chemical
- the property value or values from a given reference cannot be used because they are suspect or
- the EPA specifies that a value be calculated

3.1 RfC to RfD_{inhal}

SCDM contains RfD values for oral toxicity and RfC values for inhalation toxicity that are used to determine HTF values and screening concentration benchmarks. SCDM must convert RfC to RfD_{inhal}, for use in these determinations. RfC values are converted from concentrations into inhalation dosages (RfD_{inhal}) values for determining HTF values using the following equation:

$$RFD_{inhal} = \frac{RFC \times IR \times AR}{BM} \tag{1}$$

Where:

 RFD_{inhal} = Calculated Reference Dose in Air (mg/kg-day)

RFC = Reference Concentration in Air (mg/m³)

IR = Inhalation Rate (20 m³/day)

AR = Absorption (100% assumed unless otherwise specified)

BM = Adult Body Mass (70 kg)

Equation (1) is used to convert RfCs to inhalation RfDs. The resulting RfD_{inhal} values are used to determine HTF values (see HRS Section 2.4.1.1, Table 2-4 [40 CFR Part 300]). If the reference source used to provide the RfD or RfC does not provide a corresponding absorption, it is assumed to be 100.

3.2 IUR to Inhalation Slope Factor

SCDM contains slope factors for oral toxicity and IUR values for inhalation toxicity. IUR values are converted into inhalation slope factors (SF_{inhal}) for use in determining HTF values. SCDM converts IUR values to calculated SF_{inhal} before assigning HTF values, using the following equation:

$$SF_{inhal} = \frac{IUR \times BM \times CF}{IR \times AR} \tag{2}$$

Where:

SFinhal = Cancer Slope Factor (mg/kg-day)⁻¹

IUR = Inhalation Unit Risk $(\mu g/m^3)^{-1}$

BM = Adult Body Mass (70 kg)

CF = Conversion Factor (1,000 µg/mg)

IR = Inhalation Rate (20 m³/day)

AR = Absorption (100% assumed unless otherwise specified)

Equation (2) is used to convert the IUR value to an inhalation cancer SF, and the resulting inhalation cancer SF is evaluated with a corresponding WOE (see Section 2.2.2.1 above) to assign an HTF value based on HRS Table 2-4 (40 CFR Part 300).

3.3 Using ED10 to estimate a Slope Factor for either oral or inhalation pathways

SCDM uses slope factors and IUR values to determine human toxicity factor values and screening concentration benchmarks. In cases where a slope factor and/or IUR is not available for a substance, SCDM uses ED10 values, when available, to calculate oral and inhalation slope factors (SF_{oral} and SF_{inhal}), as follows:

$$SF_{oral} = 1 / (6 * ED10_{oral})$$
 (3)

$$SF_{inhal} = 1 / (6 * ED10_{inhal}) \tag{4}$$

3.4 Volatilization Half-Life

SCDM estimates the volatilization half-life in surface water for organic substances using Equation 5 (presented as Equation 15-12 in the "Handbook of Chemical Property and Estimation Methods," Lyman, *et al.*¹ In this method, the volatilization half-life $(T_{1/2})$ can be expressed as follows:

$$T_{1/2} = \left[\frac{Z \times \ln 2}{K_L \text{ hr}} \right] \tag{5}$$

Where:

Z = Mean water body depth (cm)

 K_L = Overall liquid-phase mass transfer coefficient

 $\ln 2 = \text{Natural logarithm of 2} (\sim 0.693147)$

The following expression gives the overall liquid-phase mass transfer coefficient:

$$K_{L} = \frac{(H/RT)k_{g} \times k_{l}}{(H/RT)k_{g} + k_{l}} cm/hr$$
(6)

Where:

H = Henry's Law constant (atm m / mol)

R = Universal gas constant $(8.2 \times 10^{-5} \text{ atm m}^3/\text{mol K})$

 $T = Temperature (K; ^{\circ}C + 273)$

 $k_g = Gas$ -phase exchange coefficient

 $k_1^s = \text{Liquid-phase exchange coefficient}$

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound.

• If MW is <65 g/mol, the following equation is used:

$$k_g = 3,000 \times (18 / MW)^{1/2} \text{ cm/hr}$$
 (7)

• If MW is \geq 65 g/mol, the following equation is used:

¹ Thomas, R.G. 1990. "Volatilization from Water." In Handbook of Chemical Property Estimation Methods. W.J. Lyman, W.F. Reehl, D.H. Rosenblatt, Eds. American Chemical Society, Washington, DC, 15:9–28. 0-ISBN 8412-1761-0.

$$k_{g} = 1,137.5 \times (V_{wind} + V_{curr})(18 / MW)^{1/2} cm/hr$$

$$\underline{Where}:$$

$$V_{wind} = Wind velocity (m/sec)$$

$$V_{curr} = Current velocity (m/sec)$$
(8)

The liquid-phase exchange coefficient also depends on the molecular weight of the compound.

• If MW is <65 g/mol, the following equation is used:

$$k_1 = 20 \times (44 / MW)^{1/2} \text{ cm/hr}$$
 (9)

• If MW is \ge 65 g/mol, the expression also depends on the wind and current velocities; the following equation is used when V_{wind} is \le 1.9 m/sec and MW is \ge 65 g/mol:

$$k_1 = 23.51 \times (V_{\text{curr}}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} \text{ cm/hr}$$
 (10)

The following equation is used when V_{wind} is >1.9 m/sec and \leq 5 m/sec, and MW is \geq 65 g/mol:

$$k_1 = 23.51 \times (V_{\text{curr}}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} e^{0.526(V_{\text{wind}} - 1.9)} \text{cm/hr}$$
(11)

No liquid-phase exchange coefficient equation is provided in Thomas (1990) for wind velocities >5 m/sec.

Combining Equations (5), (6), (7), and (9) into a single equation for estimating volatilization half-life ($T_{1/2}$) for compounds with MW <65 g/mol gives the following equation:

$$T_{1/2} = Z \times \ln 2 \times \{ [(1/20) \times (MW/44)^{1/2}] + [(RT/H \times 3000) \times (MW/18)^{1/2}] \} \text{ hr}$$
 (12)

The following equation, combining Equations (5), (6), (8), and (10), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW \geq 65 g/mol if the wind velocity is \leq 1.9 m/sec:

$$\begin{split} T_{1/2} &= Z \times ln \, 2 \times \{ [(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] \\ &+ [(RT/H \times 1,\!137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}] \} \ hr \quad (13) \end{split}$$

The following equation, combining Equations (5), (6), (8), and (11), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW \geq 65 g/mol if the wind velocity is \geq 1.9 m/sec and \leq 5 m/sec:

$$T_{1/2} = Z \times \ln 2 \times \{ [(Z^{0.673}/23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] e^{0.526(1.9 - V_{wind})} + [(RT/H \times 1,137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}] \} \text{ hr}$$
(14)

If H is <10⁻⁷ atm·m /mol, the substance is less volatile than water, and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, p. 15-15), and no volatilization half-life is estimated for rivers or lakes.

3.4.1 Volatilization Half-Life for Rivers, Oceans, Coastal Tidal Waters and the Great Lakes

To calculate the volatilization half-life for rivers, oceans, coastal tidal waters and the Great Lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 1 m/sec. Using these values, Equations (12) and (14) reduce to the following:

• If MW <65 g/mol:

$$T_{1/2} = 2.89 \times \{ [0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}] \}$$
 days (15)

• If MW ≥65 g/mol:

$$T_{1/2} = 2.89 \times \{ [0.185 \times (MW/32)^{1/2}] + [(3.6 \times 10^{-6} / H) \times (MW/18)^{1/2}] \}$$
 days (16)

Where:

 $H = Henry's Law Constant (atm \cdot m^3/mol)$

MW = Molecular Weight (g/mol)

3.4.2 Volatilization Half-Life for Lakes

To calculate the volatilization half-life for lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 0.05 m/sec. Using these values, Equations (12) and (13) reduce to the following:

• If MW <65 g/mol:

$$T_{1/2} = 2.89 \times \{ [0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}] \}$$
 days (17)

• If MW ≥65 g/mol:

$$T_{1/2} = 2.89 \times \{ [0.185 \times (MW/32)^{1/2}] + [(3.9 \times 10^{-6} / H) \times (MW/18)^{1/2}] \}$$
 days (18)

Where:

 $H = Henry's Law Constant (atm \cdot m^3/mol)$

MW = Molecular Weight (g/mol)

3.5 Overall Half-Lives

3.5.1 Overall Half-Lives for Non-radionuclides

Overall half-lives are estimated for non-radioactive substances, in rivers and lakes, as follows:

$$HALF_LAK = \frac{1}{\frac{1}{HHALFL} + \frac{1}{BHALFL} + \frac{1}{PHALFL} + \frac{1}{VHALFL}}$$
(19)

Where:

HHALFL = Hydrolysis half-life in lakes

BHALFL = Biodegradation half-life in lakes

PHALFL = Photolysis half-life in lakes

VHALFL = Volatilization half-life in lakes

$$HALF_RIV = \frac{1}{\frac{1}{HHALFR} + \frac{1}{BHALFR} + \frac{1}{PHALFR} + \frac{1}{VHALFR}}$$
(20)

Where:

HHALFR = Hydrolysis half-life in rivers

BHALFR = Biodegradation half-life in rivers

PHALFR = Photolysis half-life in rivers

VHALFR = Volatilization half-life in rivers

3.5.2 Overall Half-Lives for Radionuclides

SCDM estimates overall half-lives of radionuclides in rivers and lakes as follows (this calculation is similar to the equation used for non radioactive substances, but considers only radioactive half life and volatilization half life):

$$HALF_R_LAK = \frac{1}{\frac{1}{RHALFL} + \frac{1}{VHALFL}}$$
(21)

Where:

RHALFL = Radioactive half-life in lakes

VHALFL = Volatilization half-life in lakes

$$HALF_R_RIV = \frac{1}{\frac{1}{RHALFR} + \frac{1}{VHALFR}}$$
(22)

Where:

RHALFR = Radioactive half-life in rivers

VHALFR = Volatilization half-life in rivers

3.6 Soil Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{oc})

In the evaluation of the ground water migration pathway, a hazardous substance that does not meet the criteria for an observed release is assigned a mobility factor value from HRS Table 3-8 (Ground Water Mobility Factor Values) based on its K_d value and its water solubility value. K_d values that are not available in the references listed in Section 2.3.4 of this methodology document are calculated as detailed below:

HRS Section 3.2.1.2 (Mobility) states:

For any hazardous substance that does not meet the criteria for an observed release by chemical analysis to at least one of the aquifers, assign that hazardous substance a mobility factor value from Table 3-8 for the aquifer being evaluated, based on its water solubility and distribution coefficient (K_d) For any hazardous substance that is organic and that does not meet the criteria for an observed release by chemical analysis, establish a distribution coefficient for that hazardous substance as follows:

Estimate K_d range for the hazardous substance using the following equation:

$$K_{d} = (K_{OC})(f_{S}) \tag{23}$$

Where:

 K_{OC} = Soil-water partition coefficient for organic carbon for the hazardous substance

f_s = Sorbent content (fraction of clays plus organic carbon) in the subsurface

- Use f_S values of 0.03 and 0.77 in the above equation to establish the upper and lower values of the K_d range for the hazardous substance.
- Calculate the geometric mean of the upper and lower K_d range values. Use
 this geometric mean as the distribution coefficient in assigning the hazardous
 substance a mobility factor value from [HRS] Table 3-8.

When a K_{OC} is not available to calculate K_d values, SCDM uses the Log P or Log K_{OW} to estimate K_{OC} values. To perform this calculation, SCDM uses the relationship determined by Di'Toro (1985) for semi-volatile organic compounds:

$$Log K_{OC} = 0.00028 + (0.983 Log K_{OW})$$
 (24)

For volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides, SCDM uses the relationship derived in the Soil Screening Guidance Technical Background Document (EPA, 1996):

$$Log K_{OC} = 0.0784 + (0.7919 Log K_{OW})$$
 (25)

3.7 Water solubility for metals

If a water solubility value is not available for metal substances, it is calculated as the geometric mean of the highest water solubility and lowest water solubility of substances containing the metal, using the following equation:

Geometric Mean Solubility =
$$\sqrt{\text{(low water solubility)} \times \text{(high water solubility)}}$$
 (26)

4.0 SCREENING CONCENTRATION BENCHMARKS

Section 4 details the equations and exposure assumptions that are used to determine screening concentration benchmarks for the substances contained in SCDM. The sources of data and determination of the substance-specific values used in these equations are detailed in Sections 2.0 and 3.0 of this methodology document.

4.1 Screening Concentration Benchmarks for the Air Migration Pathway

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway. The benchmarks use exposure parameters and factors that represent Reasonable Maximum Exposure (RME) conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund*, *Part B* (1991) and *Risk Assessment Guidance for Superfund*, *Part F* (2009). General equations are provided in Section 4.1.1 (non-carcinogenic benchmarks) and Section 4.1.2 (carcinogenic benchmarks). An equation specific for asbestos is provided in Section 4.1.3. Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and trichloroethylene (TCE), are provided in Section 4.1.4; these equations are taken from EPA's *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.1.5.

4.1.1 Non-carcinogenic – Air, Inhalation

$$SC_{nc-air} = \frac{THQ \times (AT \times ED) \times \left(\frac{1000 \ \mu g}{mg}\right)}{EF \times ED \times ET \times \left(\frac{1 \ day}{24 \ hours}\right) \times \frac{1}{RfC}}$$
(27)

Where:

 SC_{nc-air} = Air Inhalation Screening Concentration, Non-Carcinogenic ($\mu g/m^3$)

THQ = Target hazard quotient (=1), unitless

AT = Averaging time (365 days/year)

ED = Exposure duration (30 years)

EF = Exposure frequency (350 days/year)

ET = Exposure time (24 hours/day)

RfC = Inhalation reference concentration (mg/m³)

Using the exposure assumptions listed above, Equation (27) can be simplified as:

$$SC_{nc-air} = 1042.857 \times RfC \tag{28}$$

4.1.2 Carcinogenic – Air, Inhalation

$$SC_{c-air} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times \left(\frac{1 \ day}{24 \ hours}\right) \times IUR}$$
(29)

Where:

 SC_{c-air} = Air Inhalation Screening Concentration, Carcinogenic ($\mu g/m^3$)

TR = Target risk (1 x 10⁻⁶) (unitless) AT = Averaging time (365 days/year) LT = Lifetime (70 years) ED = Exposure duration (30 years) EF = Exposure frequency (350 days/year) ET = Exposure time (24 hours/day) IUR = Inhalation unit risk (μ g/m³)⁻¹

Using the exposure assumptions listed above, Equation (29) can be simplified as:

$$SC_{c-air} = \frac{2.433 \times 10^{-6}}{IUR} \tag{30}$$

4.1.3 Carcinogenic – Air, Inhalation – Asbestos

$$SC_{c-air-asbestos}$$
 (fibers/mL) = $TR / (IUR \times TWF)$ (31)

Where:

 $SC_{c-air-asbestos}$ = Air Inhalation Screening Concentration, Carcinogenic, Asbestos (fibers/mL)

TR = Target risk (1 x 10^{-6}) (unitless) IUR = Inhalation Unit Risk (fibers/mL)⁻¹

TWF = Time Weighting Factor = 350/365 = 0.96

4.1.4 Carcinogenic through a Mutagenic Mode of Action – Air, Inhalation

$$SC_{mu-air} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left(\frac{1 \ day}{24 \ hours}\right) \times \left[\left(ED_{0-2} \times IUR \times 10\right) + \left(ED_{2-6} \times IUR \times 3\right)\right]}$$
(32)

 $+\left(ED_{6-16}\times IUR\times 3\right)+\left(ED_{16-30}\times IUR\times 1\right)]$

<u>Where</u>:

 $SC_{mu-air} = Air Inhalation Screening Concentration, Carcinogenic – Mutagenic Mode of Action (<math>\mu g/m^3$)

TR = Target risk (1 x 10⁻⁶) (unitless)

AT = Averaging time (365 days/year)

LT = Lifetime (70 years)

 ED_{0-2} = Exposure duration (2 years)

 ED_{2-6} = Exposure duration (4 years)

 ED_{6-16} = Exposure duration (10 years)

 ED_{16-30} = Exposure duration (14 years)

EF = Exposure frequency (350 days/year)

ET = Exposure time (24 hours/day) $UP = \text{Inhelation unit risk } (ug/m^3)^{-1}$

IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (32) can be simplified as:

$$SC_{mu-air} = \frac{9.605 \times 10^{-7}}{IUR} \tag{33}$$

4.1.4.1 Vinyl Chloride – Air, Inhalation

$$SC_{mu-vc} = \frac{TR}{IUR + \left\lceil \frac{IUR \times EF \times ED \times ET \times (1 \ day / 24 \ hours)}{(AT \times LT)} \right\rceil}$$
(34)

Where:

 SC_{mu-vc} = Air Inhalation Screening Concentration, Vinyl Chloride ($\mu g/m^3$)

TR = Target risk (1 x 10⁻⁶)

AT = Averaging time (365 days/year)

LT = Lifetime (70 years)

ED = Exposure duration (30 years)

EF = Exposure frequency (350 days/year)

ET = Exposure time (24 hours/day) IUR = Inhalation unit risk (μ g/m³)⁻¹

Using the exposure assumptions listed above, Equation (34) can be simplified as:

$$SC_{mu-vc} = \frac{7.090 \times 10^{-7}}{II/R} \tag{35}$$

4.1.4.2 Trichloroethylene – Air, Inhalation

The following three steps are used to calculate an air inhalation cancer screening concentration benchmark for TCE.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney IUR and the mutagenic equation provided below.

$$SC_{mu-tce} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1 \text{ day/24 hours}) \times [(ED_{0-2} \times IUR_{kidney} \times 10) + (ED_{2-6} \times IUR_{kidney} \times 3)} + (ED_{6-10} \times IUR_{kidney} \times 3) + (ED_{16-30} \times IUR_{kidney} \times 1)]$$
(36)

Where:

 SC_{mu-tce} = Air Inhalation Screening Concentration, Carcinogenic–Mutagenic Mode of Action ($\mu g/m^3$)

TR = Target risk (1 x 10⁻⁶) (unitless)

AT = Averaging time (365 days/year)

LT = Lifetime (70 years)

 ED_{0-2} = Exposure duration (2 years)

 ED_{2-6} = Exposure duration (4 years)

 ED_{6-16} = Exposure duration (10 years)

 ED_{16-30} = Exposure duration (14 years)

EF = Exposure frequency (350 days/year)

ET = Exposure time (24 hours/day)

 IUR_{kidney} = Inhalation unit risk, kidney (µg/m³)⁻¹

Using the exposure assumptions listed above, Equation (36) can be simplified as:

$$SC_{m-air} = 9.61 \times 10^{-7} / IUR_{kidney}$$
 (37)

Step 2. A cancer SC is calculated using the non-Hodgkin's lymphoma (NHL) and liver cancer IUR and the cancer equation provided below.

$$SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1 \ day/24 \ hours) \times IUR_{NHL and Liver}}$$
 (38)

Where: $SC_{c\text{-tce}}$ = Air Inhalation Screening Concentration, Carcinogenic (μg/m³) = Target risk (1×10^{-6}) (unitless) TR= Averaging time (365 days/year) ATLT= Lifetime (70 years) = Exposure duration (30 years) EDEF= Exposure frequency (350 days/year) ET= Exposure time (24 hours/day) = Inhalation unit risk, NHL and liver (µg/m³)⁻¹ IUR_{NHL and liver}

Using the exposure assumptions listed above, Equation (38) can be simplified as:

$$SC_{c-air} = 2.44 \times 10^{-6} / IUR_{NHL and liver}$$
 (39)

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations calculated in Steps 1 and 2 above is then generated, and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{mu-c-tce} = \frac{1}{\left(\frac{1}{SC_{m-air}}\right) + \left(\frac{1}{SC_{c-air}}\right)} \tag{40}$$

Substituting the simplified equations provided above, the following is an alternative equation for calculating Step 3 results:

$$SC_{mu-c-tce} = \frac{1}{1.04 \times 10^6 IUR_{kidney} + 4.10 \times 10^5 IUR_{NHL and Liver}}$$
(41)

4.1.5 Carcinogenic – Air, Inhalation, Radionuclides

$$SC_{c-air-rad} = \frac{TR}{ETx \left(\frac{1 \text{ day}}{24 \text{ hr}}\right) x \text{ } EFx EDx SF_{i}x IFA_{r-adj}}$$
(42)

$$\frac{Where:}{IFA_{r-adj}} = \frac{(IRA_c \times ED_c + IRA_{r-a} \times ED_{r-a})}{ED}$$

SC_{e-air-rad} = Air inhalation screening concentration benchmark – radiochemical (pCi/m³)

SF_i = Slope factor – inhalation, radiochemical – substance specific (pCi)⁻¹

TR = Target risk (1 x 10^{-6}), unitless

ET = Exposure time - resident (24 hours/day)

EF = Exposure frequency – resident (350 days/year)

ED = Exposure duration - resident (30 years)

 $IRA_c = Inhalation rate - resident child (10 m³/day)$

 ED_c = Exposure duration – resident child (6 years)

 ED_{r-a} = Exposure duration – resident adult (24 years)

 $IRA_{r-a} = Inhalation rate - resident adult (20 m³/day)$

IFA_{r-adj} = Age-adjusted inhalation factor (18 m³/day)

Using the exposure assumptions listed above, Equation (42) can be simplified as:

$$SC_{c-air-rad} = 5.29 \times 10^{-12} / SF_i$$
 (43)

4.2 Screening Concentration Benchmarks for the Soil Exposure Pathway

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund*, *Part B* (1991). General equations are provided in Section 4.2.1 (non-carcinogenic benchmarks) and Section 4.2.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.2.3; these equations are taken from EPA's *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.2.4. When determining soil ingestion screening concentration benchmarks for arsenic, the SF and RfD are multiplied by a relative bioavailability adjustment (RBA) factor of 0.6 (EPA *Guidance for Evaluating the Oral Bioavailability of Metals in Soils for Use in Human Health Risk Assessment*).

4.2.1 Non-carcinogenic – Soil, Ingestion

$$SC_{res-sol-nc-ing} = \frac{THQ \times AT \times ED_C \times BM_C}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRS_C \times \frac{10^{-6} \, kg}{mg}}$$
(44)

Where:

 $SC_{res-sol-nc-ing}$ = Soil Screening Concentration, Non-Carcinogenic (mg/kg)

RfD = Oral reference dose (in mg/kg-day)

AT = Averaging time – resident (365 days/year)

 BM_c = Body mass – child (= 15 kg)

 ED_c = Exposure duration – resident child (= 6 years)

EF = Exposure frequency – resident (= 350 days/year)

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (44) can be simplified as:

$$SC_{res-sol-nc-ing} = 78214.29 \times RfD \tag{45}$$

4.2.2 Carcinogenic – Soil, Ingestion

$$SC_{res-sol-ca-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6} \, kg}{mg}}$$
(46)

<u>Where</u>:

 $SC_{res-sol-ca-ing}$ = Soil Screening Concentration, Carcinogenic (mg/kg)

IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c}\right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BM_a}\right]$$

SF = Chronic oral cancer slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_c = Exposure duration – resident child (= 6 years)

 ED_r = Exposure duration – resident (= 30 years)

 IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

 BM_a = Body mass – adult (= 70 kg)

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (46) can be simplified as:

$$SC_{res-sol-ca-ing} = \frac{0.64}{SF} \tag{47}$$

4.2.3 Carcinogenic through a Mutagenic Mode of Action – Soil, Ingestion

$$SC_{res-sol-mu-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFSM \times \frac{10^{-6} \, kg}{mg}}$$
(48)

Where:

 $SC_{res-sol-mu-ing}$ = Soil Screening Concentration, Carcinogenic – Mutagenic Mode of Action (mg/kg) IFSM = Mutagenic soil ingestion rate – resident, age adjusted [= (489.5 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRS_c \times 10}{BM_a}\right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BM_a}\right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-30} \times IRS_a \times 1}{BM_a}\right)$$

SF = Chronic oral cancer slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_{0-2} = Exposure duration – resident ages 0-2 (= 2 years)

 ED_{2-6} = Exposure duration – resident ages 2-6 (= 4 years)

 ED_{6-16} = Exposure duration – resident ages 6-16 (= 10 years)

 ED_{16-30} = Exposure duration – resident ages 16-30 (= 14 years)

 IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

 $BM_a = Body mass - adult (= 70 kg)$

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (48) can be simplified as:

$$SC_{res-sol-mu-ing} = \frac{0.149}{SF} \tag{49}$$

4.2.3.1 Vinyl Chloride - Soil, Ingestion

$$SC_{res-sol-ca-vc-ing} = \frac{TR}{\left[\frac{SF \times EF \times IFS \times \frac{10^{-6} \, kg}{mg}}{AT \times LT}\right] + \left(\frac{SF \times IRS_C \times \frac{10^{-6} \, kg}{mg}}{BM_C}\right]}$$
(50)

Where:

SC_{res-sol-ca-vc-ing} = Soil Screening Concentration, Vinyl Chloride (mg/kg)

IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c}\right) + \left\lceil \frac{(ED_r - ED_c) \times IRS_a}{BM_a} \right\rceil$$

SF = Chronic oral cancer slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_c = Exposure duration – child (= 6 years)

 ED_r = Exposure duration – resident (= 30 years)

 IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

$$BM_a$$
 = Body mass – adult (= 70 kg)
 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (50) can be simplified as:

$$SC_{res-sol-ca-vc-ing} = \frac{0.067}{SF} \tag{51}$$

4.2.3.2 Trichloroethylene (TCE) – Soil, Ingestion

The following three steps were used to calculate a soil screening concentration benchmark reflecting exposure only via ingestion.

<u>Step 1</u>. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the mutagenic equation provided below.

$$SC_{sol-mu-tce-ing} = \frac{TR \times AT \times LT}{SF_{kidney} \times EF \times IFSM \times \frac{10^{-6} \, kg}{mg}}$$
(52)

Where:

SC_{-sol-mu-tce-ing} = Soil Screening Concentration, Mutagenic (mg/kg)

IFSM = Mutagenic soil ingestion rate-resident, age adjusted [=(489.5 mg-year)/(kg-day)], calculated as:

$$= \left(\frac{ED_{o-2} \times IRS_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-30} \times IRS_a \times 1}{BM_a}\right)$$

 SF_{kidney} = Chronic oral slope factor, kidney (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_{0-2} = Exposure duration – resident ages 0-2 (= 2 years)

 ED_{2-6} = Exposure duration – resident ages 2-6 (= 4 years)

 ED_{6-16} = Exposure duration – resident ages 6-16 (= 10 years)

 ED_{16-30} = Exposure duration – resident ages 16-30 (= 14 years)

 IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

 BM_a = Body mass – adult (= 70 kg)

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (52) can be simplified as:

$$SC_{soil-mu-tce-ing} = \frac{0.149}{SF_{kidney}} \tag{53}$$

Step 2. A cancer screening concentration (SC) is calculated using the NHL and liver cancer slope factor and the cancer equation provided below.

$$SC_{sol-ca-tce-ing} = \frac{TR \times AT \times LT}{SF_{NHL \ and \ Liver} \times EF \times IFS \times \frac{10^{-6} \ kg}{mg}}$$
(54)

Where:

 $\overline{SC_{-sol-ca-tce-ing}}$ = Soil Screening Concentration, Carcinogenic (mg/kg) IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BM_c}\right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BM_a}\right]$$

SF_{NHL} and liver = Chronic oral cancer slope factor, NHL and liver (mg/kg-day)⁻¹

= Target risk (= 1×10^{-6})

= Averaging time – resident (= 365 days/year) AT

= Lifetime (= 70 years) LT

EF= Exposure frequency – resident (= 350 days/year)

 ED_c = Exposure duration – child (= 6 years)

= Exposure duration – resident (= 30 years) ED_r

= Resident soil ingestion rate – adult (= 100 mg/day) IRS_a

 IRS_c = Resident soil ingestion rate – child (= 200 mg/day)

= Body mass - adult (= 70 kg) BM_a

= Body mass - child (= 15 kg) BM_c

Using the exposure assumptions listed above, Equation (54) can be simplified as:

$$SC_{soil-ca-tce-ing} = \frac{0.64}{SF_{NHI, and Liver}}$$
 (55)

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations, via oral ingestion, calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{soll-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{soil-ca-ing}}\right) + \left(\frac{1}{SC_{soil-mu-ing}}\right)}$$
(56)

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative equation for calculating Step 3 results:

$$SC_{soll-ca-mu-tce-ing} = \frac{1}{1.56 SF_{NHL and Liver} + 6.71 SF_{kidney}}$$
(57)

4.2.4 Carcinogenic - Soil, Radionuclides

1) Oral

$$SC_{soll-ca-rad} = \frac{TR x t_r x \lambda}{\left((1 - e^{-\lambda t_r}) x SF_s x IFS_{r-adj} x EF_r x ED_r x \left(\frac{g}{1000mg} \right) \right)}$$
(58)

Where:

IFS_r-adj
$$ED$$
 $SC_{c-sol-rad}$ $=$ Soil cancer screening concentration benchmark – radiochemical (pCi/g) SF_s $=$ Slope factor – soil, radiochemical – substance specific (pCi) $^{-1}$ IFS_{r-adj} $=$ Resident soil ingestion factor (mg/ day) TR $=$ Target risk (1 x 10^{-6}) t_r $=$ Time (30 years) λ $=$ Lamba – substance specific EF $=$ Exposure frequency – resident (350 days/year) ED $=$ Exposure duration – resident (30 years) IRS_a $=$ Soil ingestion rate – adult (100 mg/day) IRS_c $=$ Soil ingestion rate – child (200 mg/day) ED_c $=$ Exposure duration – resident child (6 years) ED_{r-a} $=$ Exposure duration – resident adult (24 years)

Using the exposure assumptions listed above, Equation (58) can be simplified as:

$$SC_{c\text{-sol-rad}} = 2.38 \times 10^{-11} \times \lambda / [(1 - e^{-30\lambda}) \times SF_s]$$
 (59)

2) External Exposure (gamma emitters)

$$SC_{ext-rad} = \frac{TR \times t_r \times \lambda}{(1 - e^{-\lambda t_r}) \times SF_{ext} \times ACF \times EF \times \left(\frac{1 \text{ year}}{365 \text{ davs}}\right) \times ED \times \left[ET_{r-o} + \left(ET_{r-i} \times GSF_i\right)\right]}$$
(60)

```
Where:
SC_{ext-rad}
            = Screening concentration benchmark – radiochemical, external (pCi/g)
            = Slope factor – external exposure – substance specific) (pCi)<sup>-1</sup>
SFext
TR
            = Target risk (= 1 \times 10^{-6})
            = Time (30 years)
tr
λ
            = Lamba – substance specific
            = Euler's number (= 2.718281828)
e
ACF
            = Area correction factor – substance specific
EF
            = Exposure frequency – resident (350 days/year)
ED
            = Exposure duration – resident (30 years)
            = Exposure duration – resident child (6 years)
ED_c
ED_{r-a}
            = Exposure duration – resident adult (24 years)
```

 ET_{r-o} = Exposure time – resident outdoor (0.073 hr/hr) ET_{r-i} = Exposure time – resident indoor (0.684 hr/hr) GSF_i = Gamma shielding factor – indoor (0.4), unitless IRS_c = Soil ingestion rate – child (200 mg/day)

Using the exposure assumptions listed above, Equation (60) can be simplified as:

$$SC_{ext-rad} = \frac{3.01 \times 10^{-6} \times \lambda}{[(1 - e^{-30\lambda}) \times SF_{ext} \times ACF]}$$
(61)

4.3 Screening Concentration Benchmarks for the Ground Water and Drinking Water Pathways

The following equations are used to determine water ingestion screening concentration benchmarks. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.3.1 (non-carcinogenic benchmarks) and Section 4.3.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 4.3.3; these equations are taken from EPA's *Handbook for Implementing the Supplemental Cancer Guidance at Waste and Cleanup Sites*. Equations used for radionuclides are provided in Section 4.3.4.

4.3.1 Non-carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water-nc-ing} = \frac{THQ \times AT \times ED_C \times BM_C \times 1000 \ \mu g/mg}{EF \times ED_C \times \left(\frac{I}{RfD}\right) \times IRW_C}$$
(62)

Where:

 $SC_{water-nc-ing}$ = Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (µg/L)

RfD = Oral reference dose (in mg/kg-day)

AT = Averaging time – resident (365 days/year)

 BM_c = Body mass – child (= 15 kg)

 ED_c = Exposure duration – child (= 6 years)

EF = Exposure frequency – resident (= 350 days/year)

 IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

THO = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (62) can be simplified as:

$$SC_{water-nc-ing} = 15642.86 \times RfD$$
 (63)

4.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water-ca-ing} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF \times EF \times IFW}$$
(64)

Where:

 $SC_{water-ca-ing}$ = Ground Water/Drinking Water Screening Concentration, Carcinogenic (µg/L)

IFW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BM_c}\right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BM_a}\right]$$

SF = Chronic oral slope factor $(mg/kg-day)^{-1}$

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_c = Exposure duration – child (= 6 years)

 ED_r = Exposure duration – resident (= 30 years)

 IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)

 IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

 BM_a = Body mass – adult (= 70 kg)

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (64) can be simplified as:

$$SC_{water-ca-ing} = \frac{0.0672}{SF} \tag{65}$$

4.3.3 Carcinogenic through a Mutagenic Mode of Action – Ground Water and Drinking Water, Ingestion

$$SC_{water-mu-ing} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF \times EF \times IFWM}$$
 (66)

Where:

 $SC_{water-mu-ing}$ = Ground Water/Drinking Water Screening Concentration, Mutagenic (µg/L)

IFWM = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (3.39 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-30} \times IRW_a \times 1}{BM_a}\right)$$

SF = Chronic oral slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_{0-2} = Exposure duration – resident ages 0-2 (= 2 years)

 ED_{2-6} = Exposure duration – resident ages 2-6 (= 4 years)

 ED_{6-16} = Exposure duration – resident ages 6-16 (= 10 years)

 ED_{16-30} = Exposure duration – resident ages 16-30 (= 14 years) IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day) IRW_c = Drinking water ingestion rate – resident child (= 1 L/day) BM_a = Body mass – adult (= 70 kg) BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (66) can be simplified as:

$$SC_{water-mu-ing} = \frac{0.0215}{SF} \tag{67}$$

4.3.3.1 Vinyl Chloride - Ground Water and Drinking Water, Ingestion

$$SC_{res-water-ca-vc-ing} = \frac{TR}{\left[\frac{SF \times EF \times IFW \times \frac{mg}{1000 \ \mu g}}{AT \times LT}\right] + \left(\frac{SF \times IRW_C \times \frac{mg}{1000 \ \mu g}}{BM_C}\right]}$$
(68)

Where:

 $SC_{res-water-nc-ing}$ = Ground Water/Drinking Water Screening Concentration, Vinyl Chloride (μ g/L) IFW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_C}{BM_C}\right) + \left[\frac{(ED_R - ED_C) \times IRW_a}{BM_a}\right]$$

SF = Chronic oral slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_c = Exposure duration –child (= 6 years)

 ED_r = Exposure duration – resident (= 30 years)

 IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)

 IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

 BM_a = Body mass – adult (= 70 kg)

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (68) can be simplified as:

$$SC_{res-water-ca-vc-ing} = \frac{0.0123}{SF} \tag{69}$$

4.3.3.2 Trichloroethylene (TCE) – Ground Water and Drinking Water, Ingestion

The following three steps were used to calculate a drinking water screening concentration reflecting exposure only via ingestion.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the

equation provided below.

$$SC_{water-mu-tce-ing} = \frac{TR \times AT \times LT \times 1000}{SF_{kidney} \times EF \times IFWM}$$
 (70)

Where:

 $SC_{water-mu-tce-ing}$ = Drinking Water Screening Concentration, Mutagenic Mode of Action (µg/L) IFWM = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (3.39 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BM_c}\right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BM_c}\right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BM_a}\right) + \left(\frac{ED_{16-30} \times IRW_a \times 1}{BM_a}\right)$$

 SF_{kidney} = Chronic oral cancer slope factor, kidney (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

 ED_{0-2} = Exposure duration – resident ages 0-2 (= 2 years)

 ED_{2-6} = Exposure duration – resident ages 2-6 (= 4 years)

 ED_{6-16} = Exposure duration – resident ages 6-16 (= 10 years)

 ED_{16-30} = Exposure duration – resident ages 16-30 (= 14 years)

 IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)

 IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

 BM_a = Body mass – adult (= 70 kg)

 BM_c = Body mass – child (= 15 kg)

Using the exposure assumptions listed above, Equation (70) can be simplified as:

$$SC_{water-mu-tce-ing} = 0.0215 / SF_{kidnev}$$
 (71)

Step 2. A cancer SC is calculated using the NHL and liver cancer slope factor and equation provided below.

$$SC_{water-ca-tce-ing} = \frac{TR \times AT \times LT \times 1000 \ \mu g/mg}{SF_{NHL,and\ Liver} \times EF \times IFW}$$
(72)

Where:

 $SC_{water-ca-tce-ing}$ = Drinking Water Screening Concentration, Carcinogenic (µg/L)

FW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)],

calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BM_c}\right) + \left\lceil \frac{(ED_r - ED_C) \times IRW_a}{BM_a} \right\rceil$$

 $SF_{NHL \ and \ liver}$ = Chronic oral cancer slope factor, NHL and liver (mg/kg-day)⁻¹

TR = Target risk (= 1×10^{-6})

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

```
ED_c = Exposure duration – child (= 6 years)

ED_r = Exposure duration – resident (30 years)

IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)

IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

BM_a = Body mass – adult (= 70 kg)

BM_c = Body mass – child (= 15 kg)
```

Using the exposure assumptions listed above, Equation (72) can be simplified as:

$$SC_{water-ca-tce-ing} = 0.067 / SF_{NHL and liver}$$
 (73)

<u>Step 3</u>. A cumulative result of both the oral mutagenic and oral cancer screening concentrations calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and NHL and liver cancer risk.

$$SC_{water-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{water-ca-ing}}\right) + \left(\frac{1}{SC_{water-mu-ing}}\right)}$$
(74)

Substituting the simplified equations provided above for obtaining Step 1 and Step 2 results, the following is an alternative to Equation 74 for calculating Step 3 results:

$$SC_{water-ca-mu-tce-ing} = \frac{1}{14.9 \, SF_{NHL \, and \, Liver} + 46.5 \, SF_{kidney}}$$
(75)

4.3.4 Carcinogenic - Ground Water and Drinking Water, Radionuclides

$$SC_{c-water-rad} = \frac{TR}{EF_r \times ED_r \times SF_w \times IFW_{r-adj}}$$
 (76)

$$\frac{Where}{IFW_{r-adj}} = \frac{ED_e \times IRW_e + ED_{r-a} \times IRW_a}{ED_r}$$

$$SC_{c-water-rad} = \text{Drinking water screening concentration benchmark} - \text{radiochemical (pCi/L)}$$

$$SF_w = \text{Slope factor} - \text{drinking water} - \text{substance specific (pCi)}^{-1}$$

$$TR = \text{Target risk (1 x 10}^{-6}), \text{ unitless}$$

$$EF = \text{Exposure frequency} - \text{resident (350 days/year)}$$

$$ED = \text{Exposure duration} - \text{resident (30 years)}$$

$$IRW_a = \text{Water ingestion rate} - \text{adult (2 L/day)}$$

$$IRW_c = \text{Water ingestion rate} - \text{child (1 L/day)}$$

 ED_c = Exposure duration – resident child (6 years) ED_{r-a} = Exposure duration – resident adult (24 years) IFW_{r-adj} = Age-adjusted water ingestion rate (1.8 L/day)

Using the exposure assumptions listed above, Equation (76) can be simplified as:

$$SC_{c\text{-water-rad}} = 5.29 \times 10^{-11} / SF_w$$
 (77)

4.4 Screening Concentration Benchmarks for the Human Food Chain Pathway

The following equations are used to determine screening concentration benchmarks for the human food chain exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided in Section 4.4.1 (non-carcinogenic benchmarks) and Section 4.4.2 (carcinogenic benchmarks). Equations used for radionuclides are provided in Section 4.4.3.

4.4.1 Non-carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res-fsh-nc-ing} = \frac{THQ \times AT \times ED_r \times BM_a}{EF \times ED_r \times \left(\frac{1}{RfD}\right) \times IRF \times \frac{10^{-6} \, kg}{mg}}$$
(78)

Where:

SC_{res-fsh-nc-ing} = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)

RfD = Oral reference dose (in mg/kg-day)

AT = Averaging time – resident (365 days/year)

 BM_a = Body mass – adult (= 70 kg)

 ED_r = Exposure duration – resident (= 30 years)

EF = Exposure frequency – resident (= 350 days/year)

IRF = Fish ingestion rate (= $5.4 \times 10^4 \text{ mg/day}$)

THO = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (78) can be simplified as:

$$SC_{res-fsh-nc-ing} = 1350 \times RfD$$
 (79)

4.4.2 Carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res-fsh-ca-ing} = \frac{TR \times AT \times LT \times BM_{a}}{EF \times ED_{r} \times SF \times IRF \times \frac{10^{-6} \, kg}{mg}}$$
(80)

Where

SC_{res-fsh-ca-ing} = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)

SF = Chronic oral cancer slope factor (mg/kg-day)⁻¹

TR = Target risk (= 1 x 10⁻⁶)

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

 BM_a = Body mass – adult (= 70 kg)

EF = Exposure frequency – resident (= 350 days/year)

ED = Exposure duration – resident (= 30 years)

IRF = Fish ingestion rate (= $5.4 \times 10^4 \text{ mg/day}$)

Using the exposure assumptions listed above, Equation (80) can be simplified as:

$$SC_{res-fsh-ca-ing} = \frac{0.00315}{SF} \tag{81}$$

4.4.3 Carcinogenic – Human Food Chain, Fish Ingestion, Radionuclides

$$SC_{C-fish-rad} = \frac{TR}{EF_r \times ED \times SF_f \times IRF \times \frac{g}{1000 \, mg}}$$
(82)

Where:

 $SC_{c-fish-rad}$ = Human Food Chain Screening Concentration, Fish Ingestion – Radiochemical, Carcinogenic (pCi/g)

 SF_f = Slope factor – drinking water – substance specific (pCi)⁻¹

 $TR = \text{Target risk } (1 \times 10^{-6}), \text{ unitless}$

EF = Exposure frequency - resident (350 days/year)

ED = Exposure duration – resident (30 years)

 ED_c = Exposure duration – resident child (6 years)

 ED_{r-a} = Exposure duration – resident adult (24 years)

 $IRF = Fish ingestion rate (= 5.4 \times 10^4 \text{ mg/day})$

Using the exposure assumptions listed above, Equation (82) can be simplified as:

$$SC_{c-fish-rad} = 1.76 \times 10^{-12} / SF_f$$
 (83)

5.0 SCDM DATA REPORTING and APPENDICES

5.1 Data Reporting

Data are collected from the references identified in Section 2 of this document. The data are collected exactly as provided in the references and compiled into a SCDM data management tool. Once in the tool, converted values are generated to reflect the SCDM standard units for use in calculations, while the original values remain unchanged for transparency. Collected data and calculated results are maintained in the tool and are not rounded, truncated or otherwise adjusted except for purposes of reporting in SCDM Appendices A, BI and BII.

The following rules are applied for purposes of reporting SCDM data in Appendices A, BI and BII:

- Substance characterization data and data that serve as inputs to benchmark and factor value formulas are truncated and reported to two significant figures.
- Screening concentration benchmarks are truncated to the number of significant figures contained in the data input variable (i.e., RfD, RfC, IUR, or cancer slope factor) used to determine each benchmark. For example, a screening concentration benchmark determined using a cancer slope factor of 2.81E-8, will be reported to three significant figures.
- Factor values will be reported to the number of significant figures needed to support decision making as described at 40 CFR Part 300 Appendix A and 55 FR 51583.

5.2 SCDM Appendices

Appendix A of SCDM contains selected data, HRS factor values and benchmarks for each hazardous substance in SCDM (the "SCDM page reports"). Information is provided in a two-page report for each substance. Data selected for SCDM are on the first page; factor values and benchmarks are on the second page.

Figure 1 presents an example of the header that appears on the Appendix A report. The header contains the date the report was created, the substance name and synonym, and the Chemical Abstract Survey Registration Number (CAS Number) for the substance.

SUPERFUND CHEMICAL DATA MATRIX								
SCDM Data Version:	Publication Date:							
Chemical: Acenapthene	CAS Number: 000083-32-9							
Figure 1	. Page Heading							

For each substance, the first page contains all of the selected chemical data, the data units, and an acronym describing the reference source of the information. Data are divided into six functional groups: toxicity, persistence, physical characteristics, mobility, bioaccumulation and other data. The "SCDM Data Version" date in the upper left-hand corner indicates the date of data collection; the "Publication Date" indicates the date the report was generated and posted on the SCDM website at http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm.

The toxicity section (Figure 2) contains the acute, chronic, and carcinogenicity data that were compiled using the methodology described in Sections 2.2 and 2.6, and used to derive toxicity and ecotoxicity factor values.

	Т	OXICITY	
<u>Parameter</u>	Value	<u>Unit</u>	Source
Oral RfD:	6.0E-2	mg/kg/day	IRIS
Inhal RfD:		mg/kg/day	
RfC:		mg/m^3	
Oral Slope:		$(mg/kg/day)^-1$	
Oral Wt-of-Evid:			
IUR:		(mg/kg/day)^-1	
IUR Wt-of-Evid:			
Oral ED10:		mg/kg/day	
Oral ED10 Wgt:			
Oral ED10 Wgt:		mg/kg/day	
Inhal ED10 Wgt:			
Oral LD50:		mg/kg	
Dermal LD50:		mg/kg	
Gas Inhal LC50:		ppm	
Dust Inhal LC50:		mg/L	
ACUTE		-	
Fresh CMC:		μg/L	
Salt CMC:		μg/L	
CHRONIC			
Fresh CCC:		μg/L	
Salt CCC:		μg/L	
Fresh Ecol LC50:	5.0E+1	, -	ECOTOX
Salt Ecol LC50:	1.4E+2		ECOTOX
	Figure 2.	Toxicity Section	

The top half of this section contains the data used to determine the HTF value: reference dose (oral and inhalation), cancer slope factor (oral and inhalation unit risk [IUR]), ED_{10} (oral and inhalation), LD_{50} (oral and dermal) and LC_{50} (gas and dust inhalation). The bottom half of this section contains the data used to determine an ecotoxicity factor value: acute and chronic water quality criteria, CMC and CCC, for fresh and salt water as well as fresh and salt water LC_{50} values. Blank entries indicate that no value was found using the procedures and references specified.

The persistence section (Figure 3) contains the surface water persistence data compiled using the methodology described in Section 2.4. Surface water persistence factors can also be determined using the logarithm of the n-octanol/water partition coefficient (Log K_{OW} or Log P, Section 2.3) if, as specified in the HRS, this gives a higher factor value than the half-lives (or a default, if applicable).

	PERSISTE	NCE	
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Source</u>
LAKE - Halflives			
Hydrolysis:		days	
Volatility:	1.1E+2	days	THOMAS
Photolysis:	2.5E+0	days	HEDR
Biodeg:	1.0E+2	days	HEDR
Radio:		days	
RIVER - Halflives			
Hydrolysis:		days	
Volatility:	1.3E+0	days	THOMAS
Photolysis:	2.5E+0	days	HEDR
Biodeg:	1.0E+2	days	HEDR
Radio:		days	
Log Kow:	3.9E+0		EPI
	Figure 3. Persister	nce Section	

The physical characteristics section (Figure 4) contains logical "yes/no" flags that classify the substance. The "metal contain" flag indicates that the hazardous substance is a metal or metalloid and is used to determine ground water mobility and surface water persistence factors. The "organic" and "inorganic" flags are used to determine ground water mobility and bioaccumulation. The "radionuclide" flag is used to determine the HTF, the ecosystem toxicity factor and the surface water persistence factor. The radioactive element flag ("rad. element") is used to determine whether or not the HRS factors and benchmarks (second page) are printed. The gas and particulate flags are used to determine mobility and likelihood of release for the air pathway. MW is used to determine volatilization half-life.

PHYSICAL CHARACTERISTICS												
<u>Parameter</u>	<u>Value</u>											
Metal Contain:	No											
Organic:	Yes											
Gas:	Yes											
Particulate:	Yes											
Radionuclide:	No											
Rad. Element:	No											
Molecular Weight:	1.5E+2											
Density:	1.2E+0	g/mL	@ 20.00	C								
Figure	4. Physical C	haracteristic	cs Section									

The mobility section (Figure 5) contains the air and ground water mobility data compiled using the methodology described in Section 2.3. Vapor pressure and HLC are used to determine gas migration potential and gas mobility factors. HLC is also used to calculate the volatilization half-life. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor. Substance-specific water solubility is used for nonmetal and non-metalloid substances, whereas for metal-containing substances, the solubility value is the geometric mean of the available water solubilities for inorganic compounds containing the hazardous substance.

MOBILITY											
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	Source								
Vapor Press:	2.2E-3	Torr	PHYSPROP								
Henry's Law:	1.8E-4	atm-m3/mol	PHYSPROP								
Water Solub:	3.9E+0	mg/L	PHYSPROP								
Distrib Coef:	7.6E+2	ml/g	CALC								
Geo Mean Sol:		mg/L									
	Figure 5. N	lobility Section									

The bioaccumulation section (Figure 6) contains the human food chain and environmental bioaccumulation potential factor data compiled using the methodology described in Section 2.5. BCFs are collected for fresh and saltwater for the human food chain and environmental threats. Log $K_{\rm OW}$ or water solubility is used to establish bioaccumulation potential when a BCF is not available.

	BIOACCUMULATION											
<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	Source									
FOOD CHAIN												
Fresh BCF:	3.9E+2		ECOTOX									
Salt BCF:												
ENVIRONMENTAL												
Fresh BCF:	3.9E+2		ECOTOX									
Salt BCF:												
Log Kow:	3.9E+0		EPI									
Water Solub:	3.9E+0		PHYSPROP									
Geo Mean Sol:		mg/L										
Figu	re 6. Bioacc	umulation Sec	tion									

The section labeled "other data" (Figure 7) contains values for melting points and boiling points (°C) along with the associated vapor pressure (Torr), if applicable. The chemical formula is also listed here.

	OTHER DATA	ı	
Melting Point:	9.3E+1	C	
Boiling Point:	2.8E+2	C	
Formula	C12 H10		
Fig	ure 7. Other D	ata	

The class information section (Figure 8) lists parent substances for three data substitution classes: toxicity, ground water mobility and other data. The toxicity class includes all toxicity and benchmark data used to determine human or ecotoxicity factor values. The ground water mobility class includes water solubility, K_d , and geometric mean water solubility. The "other" class includes hydrolysis, biodegradation, photolysis and volatilization half-lives, as well as BCFs and Log K_{ow} . This section may also list other class-parent chemical substitutions for specific data elements.

Currently, only two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for the ground water mobility class with the elemental metal as the class parent. Radioactive isotopes may inherit data from their primary radioactive element for the ground water mobility and "other" classes.

CLASS INFORMATION										
Class	Parent Substance									
Figure	8. Class Information Section									

The second page for each substance is divided into top and bottom sections that contain factor values (Figure 9) and benchmarks (Figure 10) required by the HRS. SCDM determines factor values using HRS methodologies from selected data on the first page of the SCDM page report. The factor values are presented by exposure pathway: air, ground water, soil and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. The toxicity factor value represents human toxicity and is the same for all pathways. The air pathway gas migration factor value is used to determine likelihood of release. The surface water environmental toxicity factor values are based on fresh and saltwater ecosystem toxicity data, and the surface water persistence factor values are based on BCFs for all aquatic species. The surface water human food chain factor values are based on human toxicity and BCFs for only those aquatic species consumed by humans. For radioactive substances, human toxicity, ecosystem toxicity and surface water persistence factor values are determined as specified in Section 7 of the HRS.

		ASSIGNED	FACTOR VALUE	ES				
AIR PATI	YAW	GROUND WAT	ER PATHWAY	SOIL EXPO	SURE PATHWAY			
<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>			
Toxicity:	10	Toxicity:	10	Toxicity:	10			
Gas Mobility:	0.2000	Water Solub:	3.9E+0					
Gas Migration:	11	Distrib:	7.6E+2					
		Geo Mean Sol:						
		Liquid						
		Karst:	1.0E+0					
		Non Karst:	1.0E-2					
		Non Liq.						
		Karst:	2.0E-1					
		Non Karst:	2.0E-3					
		SURFACE	WATER PATHWA	AY				
DRINKING	WATER	HUMAN FO	OOD CHAIN	ENVIRONMENTAL				
<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>	<u>Parameter</u>	<u>Value</u>			
Toxicity:	10	Toxicity:	10	Fresh Tox:	10000			
				Salt Tox:	1000			
Persistence		Persistence		Persistence				
River:	0.4000	River:	0.4000	River:	0.4000			
Lake:	0.4000	Lake:	0.4000	Lake:	0.4000			
		Bioaccumulation		Bioaccumulation	1			
		Fresh:	500.0	Fresh:	500.0			
		Salt:	500.0	Salt:	500.0			
		Figure 9. Assigne	ed Factor Values	Section				

The benchmarks (Figure 10), like the factor values, are presented by pathway: air, ground water, soil exposure, and surface water. The surface water pathway is further subdivided by threat: drinking water, human food chain, and environmental. For HRS scoring, actual sample contaminant concentrations for a particular medium are compared to these benchmark concentrations to determine if the target will be scored as subject to Level I or Level II concentrations.

					BENCI	HMARKS						
AIR PA	THW	ΛY		ND WATE FHWAY	ER		EXPOSUI FHWAY	RE	RADIONUCLIDE			
<u>Parameter</u>	Value	<u>Unit</u>	<u>Parameter</u>	Value	<u>Unit</u>	<u>Parameter</u>	Value	<u>Unit</u>	<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	
NAAQS/ NESHAPS:		μg/m3	MCL/ MCLG:			Cancer Risk		mg/kg	MCL:		pCi/L	
Cancer Risk		μg/m3	Cancer Risk		mg/L	Non Cancer Risk	4.7E+3	mg/kg	UMTRCA:		pCi/kg	
Non Cancer Risk		μg/m3	Non Cancer Risk	9.4E-1	mg/L				CANCER RISK			
									Air:		pCI/m3	
									DW:		pCI/L	
									FC:		pCi/kg	
									Soil Ing:		pCi/kg	
									Soil GAM:		pCi/kg	
				SURFA	CE WA	TER PATHW	/AY					
DRINI	KING V	WATER		HUMA	N FOO	D CHAIN		1	ENVIRONME	NTAL		
<u>Parameter</u>	Valu	<u>ue</u> <u>Unit</u>	Param	<u>eter</u>	Valu	<u>Unit</u>	Para	<u>ameter</u>	<u>Value</u>	U	<u>nit</u>	
MCL/MCLG:		mg/	L FDAA	L:		ppm	ACI	UTE		n	ng/kg	
Cancer Risk Non Cancer		mg/	L Cance	r Risk		mg/kg	F	resh CM0	C:	m	ng/kg	
Risk	9.4E	-1 mg/	L Non C	ancer Risk	8.1E-	+1 mg/kg	S	alt CMC:				
							CHI	RONIC				
							F	resh CCC	:	μ	g/L	
							S	alt CCC:			g/L	

Appendix B is divided into two sections, Appendix B-I and B-II. Appendix B-I contains all of the factor values by exposure pathway. Factor values for non-radionuclide substances are listed first and are followed by a listing of factor values for radionuclides. Appendix B-II presents all the screening concentration benchmarks by exposure pathway. Benchmarks are provided for the drinking water/groundwater and surface water exposure pathways, followed by the air and soil exposure pathways. Benchmarks for non-radionuclide substances are provided first, followed by benchmarks for the radionuclides. Appendix C contains a cross-reference index of hazardous substance names, synonyms and CAS Numbers for substances in SCDM.

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				Ground Wat	er Mobility	,	Persistence Bioaccumulation			Facto	oxicity							
			L	iquid	Nor	n-Liquid	_ reisi	stence	Food	Chain	Envir	onment	_ Econ	oxicity	Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migratio			Part
Acenaphthene	000083-32-9	10	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	0.4	500	500	500	500	10000	1000	11	0.2	Yes	Yes
Acenaphthylene	000208-96-8	1	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	1	500	500	500	500	0	0	11	0.2	Yes	Yes
Acetone	000067-64-1	1	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.07	0.5	0.5	0.5	0.5	100	1	17	1	Yes	No
Acrolein	000107-02-8	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.07	0.07	500	500	500	500	1000	1000	17	1	Yes	No
Acrylamide	000079-06-1	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	5	5	5	5	10	10	6	0.2	Yes	Yes
Alachlor	015972-60-8	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	500	50	50	10000	100	6	0.02	Yes	Yes
Aldrin	000309-00-2	10000	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	5000	50000	50000	50000	10000	10000	11	0.02	Yes	Yes
Aluminum	007429-90-5	1000	1.0E+00	1.0E-04	1.0E+00	1.0E-04	1	1	50	50	50000	50000	100	100			No	Yes
Americium	007440-35-9	0	1.0E+00	1.0E-02			1	1	5000	500	5000	5000	0	0			No	Yes
Ammonia	007664-41-7	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.07	0.5	0.5	0.5	0.5	1000	1000	17	1	Yes	No
Aniline	000062-53-3	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	0.4	50	50	500	500	10000	10	11	1	Yes	No
Anthracene	000120-12-7	10	1.0E+00	1.0E-04	2.0E-03	2.0E-07	0.4	0.4	50000	50000	50000	50000	10000	10000	6	0.002	Yes	Yes
Antimony	007440-36-0	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	5	5	50	1	100			No	Yes
Arsenic	007440-38-2	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	500	50000	500	10	100			No	Yes
Asbestos	001332-21-4	10000	1.0E+00	1.0E-04			1	1	0.5	0.5	0.5	0.5	0	0			No	Yes
Atrazine	001912-24-9	100	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.0007	0.07	5000	5000	50000	50000	10000	10000	0	0.002	Yes	Yes
Barium	007440-39-3	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	500	500	500	1	1			No	Yes
Benz(a)anthracene	000056-55-3	1000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	10000	10000	6	0.002	Yes	Yes

Publication Date: 06/20/2014

Last Modified Date: 01/30/2014

Ground Water Mobility Bioaccumulation Persistence Ecotoxicity Liquid Non-Liquid Food Chain Environment Air Gas Air Gas MigrationMobility Gas Part Substance Name CAS Number Toxicity Karst Non-Karst Karst Non-Karst River Lake Salt Fresh Salt Fresh Salt Fresh Benzene 000071-43-2 1000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 0.4 0.4 5000 5000 5000 50000 1000 1000 17 Yes No Benzidine 000092-87-5 10000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 0.4 50 50 5000 5000 100 100 0 0.002 Yes Yes 1 10000 Benzo(a)pyrene 000050-32-8 10000 1.0E+001.0E-04 2.0E-05 2.0E-09 50000 50000 50000 50000 10000 6 0.0002 Yes Yes 0 0 Benzo(g,h,i)perylene 000191-24-2 0 1.0E+00 1.0E-04 2.0E-05 2.0E-09 50000 50000 50000 50000 No Yes Benzo(j,k)fluorene 000206-44-0 50000 10000 0.002 100 1.0E+00 1.0E-04 2.0E-03 2.0E-07 1 5000 5000 50000 10000 6 Yes Yes (Fluoranthene) Benzo(k)fluoranthene 000207-08-9 100 1.0E+001.0E-04 2.0E-05 2.0E-09 1 50000 50000 50000 50000 0 0 6 0.0002 Yes Yes Bervllium 007440-41-7 10000 1.0E+001.0E-02 1.0E+001.0E-02 1 50 50 50 50 1000 1000 No Yes Bis(2-ethylhexyl) phthalate 000117-81-7 100 1.0E+00 1.0E-04 2.0E-03 2.0E-07 50000 500 50000 5000 1000 1000 6 0.002 Yes No Boron 007440-42-8 100 1.0E+00 1.0E+00 0.5 0.5 50 50 0 0 No Yes 0 Bromodichloromethane 000075-27-4 100 1.0E+001.0E+00 1.0E+001.0E+00 0.4 50 50 50 50 0 17 Yes No 1000 1000 Butylbenzyl phthalate 000085-68-7 10 1.0E+00 1.0E-04 2.0E-01 2.0E-05 500 500 500 500 6 0.002 Yes No Cadmium 007440-43-9 10000 1.0E+00 1.0E-02 1.0E+001.0E-02 1 50000 50000 50000 50000 10000 1000 No Yes 000086-74-8 10 1.0E+00 1.0E-04 2.0E-01 2.0E-05 500 500 500 500 1000 0 0.002 Yes Yes Carbazole 1 1000 Carbon Disulfide 10 0.4 5 5 5 000075-15-0 1.0E+00 1.0E+00 1.0E+00 1.0E+00 0.4 5 100 10 17 Yes No Carbon Tetrachloride 000056-23-5 1000 1.0E+001.0E+00 1.0E+001.0E+00 0.4 50 50 500 500 100 10 17 Yes No Cesium 007440-46-2 0 1.0E+001.0E+001.0E+00 1.0E+00 5 50 5 50 0 0 No Yes 10000 10000 Chlordane 012789-03-6 1.0E+00 1.0E-04 2.0E-03 2.0E-07 1 5000 5000 50000 50000 10000 6 0.002 Yes Yes 10000 1.0E+00 2.0E-07 50000 10000 10000 11 Chlordane, alpha-005103-71-9 1.0E-04 2.0E-03 50000 50000 50000 0.02 Yes Yes

Publication Date: 06/20/2014

Last Modified Date: 01/30/2014

Ground Water Mobility Bioaccumulation Persistence Ecotoxicity Food Chain Liquid Non-Liquid Environment Air Gas Air Gas MigrationMobility Gas Part Substance Name CAS Number Toxicity Karst Non-Karst Karst Non-Karst River Lake Fresh Salt Salt Fresh Salt Fresh Chlordane, gamma-005103-74-2 10000 1.0E+00 1.0E-04 2.0E-03 2.0E-07 50000 5000 5000 50000 10000 10000 11 0.02 Yes Yes Chlorobenzene 000108-90-7 100 1.0E+00 1.0E-02 1.0E+00 1.0E-02 0.0007 0.07 50 50 5000 5000 10000 100 17 Yes No 1.0E+00 0.4 5 5 17 Chloroform 000067-66-3 100 1.0E+00 1.0E+00 1.0E+00 500 500 1000 10 Yes No 5 Chromium 007440-47-3 10000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 500 500 500 10000 1000 No Yes 1.0E+00 1.0E-04 500 500 Chromium(III) 016065-83-1 1 1.0E-04 1.0E+00 500 500 100 100 No Yes Chromium(VI) 018540-29-9 10000 1.0E+00 1.0E-02 1.0E+001.0E-02 1 5 500 5 500 100 100 No Yes 2.0E-05 5 Chrysene 000218-01-9 10 1.0E+001.0E-04 2.0E-09 1 5 5000 5000 1000 1000 0.0002 Yes Yes Cobalt 007440-48-4 10000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 50 5000 50 5000 0 0 No Yes Copper 007440-50-8 100 1.0E+00 1.0E-02 1.0E+00 1.0E-02 50000 50000 50000 50000 1000 1000 No Yes Cumene 000098-82-8 10 1.0E+00 1.0E-02 2.0E-01 2.0E-03 0.4 0.4 500 500 500 500 100 10 17 Yes No Cyanamide 10 1.0E+00 1.0E+00 0.5 0.5 0.5 100 6 0.2 000420-04-2 1.0E+00 1.0E+00 0.5 10 Yes Yes 0.5 Cyanide 000057-12-5 10000 1.0E+00 1.0E+00 1.0E+001.0E+00 0.4 0.07 0.5 0.5 0.5 1000 1000 17 Yes No DDD 000072-54-8 100 1.0E+00 1.0E-04 2.0E-03 2.0E-07 1 50000 50000 50000 50 10000 10000 6 0.002 Yes Yes **DDE** 2.0E-03 50000 50000 50000 10000 10000 0.002 Yes Yes 000072-55-9 100 1.0E+00 1.0E-04 2.0E-07 50000 6 DDT 000050-29-3 1000 1.0E+001.0E-04 2.0E-05 2.0E-09 50000 5000 50000 5000 10000 10000 0.002 Yes Yes Di-n-butyl phthalate 000084-74-2 10 1.0E+001.0E-02 2.0E-01 2.0E-03 0.4 5000 5000 50000 5000 1000 10000 6 0.02 Yes No 50000 0 0 0.0002 Di-n-octyl phthalate 000117-84-0 100 1.0E+00 1.0E-04 2.0E-03 2.0E-07 1 1 500 500 50000 Yes No 10000 1.0E+00 1.0E-04 2.0E-05 2.0E-09 50000 0 0 Dibenz(a,h)anthracene 000053-70-3 50000 50000 50000 No Yes

Publication Date: 06/20/2014

Last Modified Date: 03/14/2014 Hazardous Substance

				Ground Wate	er Mobility	,	Dorai	stence		Bioacc	cumulation		Easter	oxicity				
			L	iquid	Non	ı-Liquid	- reisi	stelice	Food	Chain	Envir	onment	_ ECOIO	oxicity	Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migration			Part
Dibenzofuran	000132-64-9	1000	1.0E+00	1.0E-04	2.0E-01	2.0E-05	0.4	1	500	500	500	500	1000	1000	11	0.2	Yes	Yes
Dibromo-3-chloropropane, 1,2-	000096-12-8	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50	50	50	50	10	10	11	1	Yes	No
Dibromoethane, 1,2-	000106-93-4	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	10	100	17	1	Yes	No
Dibutyltin	001002-53-5	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	5	5	5	5	0	0	17	1	Yes	No
Dibutyltin dichloride	000683-18-1	10000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	50	50	50	50	100	1000	17	0.2	Yes	Yes
Dichlorobenzene, 1,4-	000106-46-7	10	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	0.4	5000	5000	5000	5000	1000	1000	17	1	Yes	No
Dichloroethane, 1,1-	000075-34-3	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	0	0	17	1	Yes	No
Dichloroethane, 1,2-	000107-06-2	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	10	100	17	1	Yes	No
Dichloroethylene, 1,1-	000075-35-4	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	100	1	17	1	Yes	No
Dichloroethylene, 1,2- (Mixed Isomers)	000540-59-0	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	1	100	17	1	Yes	No
Dichloroethylene, 1,2-cis-	000156-59-2	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	0	0	17	1	Yes	No
Dichloroethylene, 1,2-trans	- 000156-60-5	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	1	1	17	1	Yes	No
Dichlorophenol, 2,4-	000120-83-2	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.0007	0.07	50	50	5000	5000	10000	100	11	0.2	Yes	Yes
Dichloropropane, 1,2-	000078-87-5	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	10	10	17	1	Yes	No
Dichloropropene, 1,3-	000542-75-6	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	0.4	50	50	50	50	1000	1000	17	1	Yes	No
Dieldrin	000060-57-1	10000	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	50000	5000	50000	50000	10000	10000	6	0.002	Yes	Yes
Diethyl phthalate	000084-66-2	1	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	500	500	500	10	100	11	0.2	Yes	No
Dimethyl phenol, 2,4-	000105-67-9	100*	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	0.4	500	500	500	500	100	1000	11	1	Yes	Yes

^{*} Value was modified since the January 2014 publication of SCDM. See Change Control documentation for details (http://www.epa.gov/superfund/sites/npl/hrsres/tools/changecontrol.pdf)

Publication Date: 06/20/2014

Last Modified Date: 01/30/2014

Ground Water Mobility Bioaccumulation Persistence Ecotoxicity Food Chain Liquid Non-Liquid Environment Air Gas Air Gas MigrationMobility Gas Part Substance Name CAS Number Toxicity Karst Non-Karst Karst Non-Karst River Lake Salt Fresh Salt Fresh Salt Fresh 5 Yes Dinitrobenzene, 1,3-000099-65-0 10000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 0.4 5 5 5 100 100 6 0.02 Yes 000123-91-1 100 1.0E+00 1.0E+00 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 No Yes Dioxane, 1,4-1 1 1 0 0.07 0.5 0.5 0 Dioxin, 1.4-000290-67-5 1.0E+00 0.4 0.5 0.5 0 No Yes Diphenylhydrazine, 1,2-000122-66-7 1000 1.0E+00 1.0E-02 1.0E+00 1.0E-02 50 50 50 50 1000 1000 6 0.02 Yes Yes Disulfoton 000298-04-4 10000 1.0E+00 2.0E-03 0.4 500 500 5000 10000 10000 0.02 1.0E-02 2.0E-01 5000 6 Yes Yes 1.0E-04 Endosulfan (I or II) 000115-29-7 100 1.0E+00 2.0E-03 2.0E-07 1 0.4 5 5000 50000 5000 10000 10000 6 0.002 Yes Yes 0.002 Yes Yes Endosulfan I 000959-98-8 100 1.0E+001.0E-04 2.0E-03 2.0E-07 1 500 500 50000 50000 10000 10000 6 Endosulfan II 033213-65-9 100 1.0E+00 1.0E-04 2.0E-03 2.0E-07 500 500 5000 5000 10000 10000 6 0.002 Yes Yes Endrin 000072-20-8 10000 1.0E+00 1.0E-04 2.0E-03 2.0E-07 5000 5000 50000 5000 10000 10000 6 0.002 Yes Yes Endrin aldehyde 007421-93-4 0 1.0E+001.0E-02 2.0E-03 2.0E-05 5000 5000 5000 5000 0 0 6 0.002 Yes Yes 0.0007 5 5 5 5 0 0 17 Ethyl chloride 000075-00-3 1 1.0E+00 1.0E+001.0E+00 1.0E+00 0.07 Yes No Ethylbenzene 000100-41-4 10 1.0E+001.0E-02 1.0E+001.0E-02 0.4 0.4 50 50 50 50 100 1000 17 Yes No Ethylene glycol monobutyl 000111-76-2 10 1.0E+00 1.0E+00 1.0E+00 1.0E+00 5 5 5 5 1 1 No No ether (EBGE) 0.4 500 500 5000 5000 1000 Fluorene 000086-73-7 100 1.0E+00 1.0E-04 2.0E-01 2.0E-05 1000 11 0.02 Yes Yes Fluorine 007782-41-4 1000 1.0E+001.0E-02 2.0E-01 2.0E-03 0.4 0.07 50000 50000 50000 50000 0 0 17 Yes No Furfural 000098-01-1 1000 1.0E+001.0E+001.0E+00 1.0E+00 0.5 0.5 0.5 0.5 100 100 11 Yes No Heptachlor 50000 50000 10000 10000 0.02 000076-44-8 1000 1.0E+00 1.0E-04 2.0E-03 2.0E-07 1 500 50000 11 Yes Yes 10000 1.0E+00 1.0E-04 2.0E-03 2.0E-07 5000 5000 5000 10000 10000 11 Heptachlor epoxide 001024-57-3 50000 0.02 Yes Yes Last Modified Date: 01/30/2014

HAZARD RANKING SYSTEM Hazardous Substance Factor Values

			Ground Water Mobility					stence						oxicity				
			L	iquid	Nor	n-Liquid	. 1 6181	Stellee	Food	Chain	Envir	onment	_ Ecoto	acity	Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt		nMobility	Gas	Part
Heptachlorodibenzo-p- dioxin	037871-00-4	0	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Heptachlorodibenzo-p-dioxin, 1,2,3,4,6,7,8-	035822-46-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Heptachlorodibenzofuran, 1,2,3,4,6,7,8-	067562-39-4	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0	6	0.0002	Yes	Yes
Heptachlorodibenzofuran, 1,2,3,4,7,8,9-	055673-89-7	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexabromobiphenyl (PBB)	036355-01-8	1	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	50000	50000	50000	50000	0	0	6	0.0002	Yes	Yes
Hexachlorobenzene	000118-74-1	1000	1.0E+00	1.0E-02	2.0E-05	2.0E-07	1	1	50000	50000	50000	50000	10000	10000	11	0.02	Yes	Yes
Hexachlorobutadiene	000087-68-3	1000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	50000	50000	50000	50000	10000	10000	17	1	Yes	No
Hexachlorocyclohexane, alpha-	000319-84-6	10000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	5000	50000	5000	50000	1000	1000	11	0.02	Yes	Yes
Hexachlorocyclohexane, beta-	000319-85-7	1000	1.0E+00	1.0E-02	2.0E-03	2.0E-05	1	1	500	500	5000	5000	1000	1000	6	0.002	Yes	Yes
Hexachlorodibenzo-p-dioxin, 1,2,3,4,7,8-	039227-28-6	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	5000	5000	5000	5000	0	0			No	Yes
Hexachlorodibenzo-p-dioxin, 1,2,3,6,7,8-	057653-85-7	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexachlorodibenzo-p-dioxin, 1,2,3,7,8,9-	019408-74-3	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexachlorodibenzofuran, 1,2,3,4,7,8-	070648-26-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexachlorodibenzofuran, 1,2,3,6,7,8-	057117-44-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexachlorodibenzofuran, 1,2,3,7,8,9-	072918-21-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hexachlorodibenzofuran, 2,3,4,6,7,8-	060851-34-5	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Hydrazine	000302-01-2	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	0.4	0.5	0.5	0.5	0.5	10000	100	11	1	Yes	No
Hydrogen sulfide	007783-06-4	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.07	0.5	0.5	0.5	0.5	1000	1000	17	1	Yes	No

Last Modified Date: 01/30/2014

NKING SYSTEM Publication Date: 06/20/2014

			Ground Water Mobility				Doro	stence						xicity				
			L	iquid	Nor	n-Liquid	_ 10151	sterice	Food	Chain	Envir	onment	_ Econ	xicity	Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migration		Gas	Part
Indeno(1,2,3-cd)pyrene	000193-39-5	1000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Iron	007439-89-6	1	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5000	5000	50000	5000	10	10			No	Yes
Lead	007439-92-1	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5000	5000	50000	5000	1000	1000			No	Yes
Lead chromate	007758-97-6	10000	1.0E+00	1.0E+00	2.0E-03	2.0E-03	1	1	50000	50000	50000	50000	0	0			No	Yes
Lindane (Hexachlorocyclohexane,	000058-89-9	10000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	50000	5000	50000	5000	10000	10000	6	0.02	Yes	Yes
Manganese	007439-96-5	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	50000	50000	50000	100	100			No	Yes
Mecoprop	000093-65-2	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	0.4	500	500	500	500	100	100	0	0.002	Yes	Yes
Mercury (elemental)	007439-97-6	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50000	50000	50000	50000	10000	10000	17	0.2	Yes	No
Methoxychlor	000072-43-5	100	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	500	50000	5000	50000	10000	10000	6	0.002	Yes	Yes
Methyl Ethyl Ketone (2-Butanone)	000078-93-3	1	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.4	0.5	0.5	0.5	0.5	1	1	17	1	Yes	No
Methyl Parathion	000298-00-0	10000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	0.4	50	50	50	50	10000	10000	6	0.002	Yes	Yes
Methyl isobutyl ketone	000108-10-1	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.4	5	5	5	5	1	1	17	1	Yes	No
Methyl tert-Butyl Ether (MTBE)	001634-04-4	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	1	1	17	1	Yes	No
Methyl-4- chlorophenoxyacetic acid,	000094-74-6	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	0.4	500	500	500	500	10000	1	0	0.002	Yes	Yes
Methylene Chloride	000075-09-2	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	500	500	1	10	17	1	Yes	No
Methylnaphthalene, 2-	000091-57-6	1000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	0.4	50000	50000	50000	50000	100	1000	11	0.2	Yes	Yes
Methylphenol, 4-	000106-44-5	10	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.0007	0.0007	50	50	50	50	100	100	11	1	Yes	No
Naphthalene	000091-20-3	1000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	0.4	50000	5000	50000	5000	1000	1000	11	0.2	Yes	Yes

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Dublication	Data:	06/20/2014
Publication	Date.	00/20/2014

			Ground Water Mobility				Dorci	stence					Ecotoxicity					
			L	iquid	Non	-Liquid	_ 1 C151	Stellee	Food	Chain	Envir	onment	_ Leotomeny		Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migratio			Part
Nickel	007440-02-0	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	5	50000	5	100	1000			No	Yes
Nitrobenzene	000098-95-3	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50	50	50	50	100	100	11	1	Yes	No
Nitrosodimethylamine, N-	000062-75-9	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.0007	0.07	0.5	0.5	0.5	0.5	1	1	11	1	Yes	No
Nitrosodiphenylamine, N-	000086-30-6	10	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	500	500	500	500	100	100	11	0.2	Yes	Yes
Octachlorodibenzo-p- Dioxin 1,2,3,4,6,7,8,9-	003268-87-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	5000	5000	50000	50000	0	0			No	Yes
Octachlorodibenzofuran 1,2,3,4, 6,7,8,9-(OCDF)	039001-02-0	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	5000	5000	0	0			No	Yes
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	040321-76-4	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Pentachlorodibenzofuran, 1,2,3,7,8-	057117-41-6	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Pentachlorodibenzofuran, 2,3,4,7,8-	057117-31-4	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0	6	0.0002	Yes	Yes
Pentachlorophenol (PCP)	000087-86-5	100	1.0E+00	1.0E-02	2.0E-01	2.0E-03	1	1	50000	5000	50000	5000	100	1000	6	0.02	Yes	Yes
Perchlorate	014797-73-0	1000	1.0E+00	1.0E+00			0.4	0.07	0.5	0.5	0.5	0.5	0	0			No	Yes
Phenanthrene	000085-01-8	1	1.0E+00	1.0E-04	2.0E-01	2.0E-05	0.4	0.4	5000	5000	50000	5000	10000	10000	11	0.02	Yes	Yes
Phenol	000108-95-2	10	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	0.4	50	50	50000	50	10000	1000	11	1	Yes	No
Plutonium	007440-07-5	0	1.0E+00	1.0E+00			1	1	50	50	500	500	0	0			No	Yes
Polychlorinated biphenyls (PCBs)	001336-36-3	10000	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	50000	50000	50000	50000	10000	10000	11	0.02	Yes	Yes
Pyrene	000129-00-0	100	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	50000	5000	50000	5000	10000	10000	6	0.002	Yes	Yes
Radium	007440-14-4	0	1.0E+00	1.0E-02			1	1	0.5	0.5	0.5	0.5	0	0			No	Yes
Radon	010043-92-2	0	1.0E+00				0.4	0.07	0.5	0.5	0.5	0.5	0	0	17	1	Yes	No

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	_		Ground Wate	er Mobility		Dorai	stence	Bioaccumulation				Facto	wiaitr					
			L	iquid	Non	ı-Liquid	Peisi	stence	Food	Chain	Envir	onment	_ Ecolo	oxicity	Air Gas	Air Gas		
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt		nMobility	Gas	Part
Selenium	007782-49-2	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	50	500	500	500	1000	100			No	Yes
Silver	007440-22-4	100	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	50	50000	50	50000	10000	10000			No	Yes
Strontium	007440-24-6	1	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	5	5	5	5	0	0			No	Yes
Styrene	000100-42-5	10	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	50	50	100	100	17	1	Yes	No
Tetrachlorobenzene, 1,2,4,5-	000095-94-3	10000	1.0E+00	1.0E-02	2.0E-03	2.0E-05	1	1	5000	5000	5000	5000	10000	1000	11	0.2	Yes	Yes
Tetrachlorodibenzo-p- dioxin	041903-57-5	0	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0			No	Yes
Tetrachlorodibenzo-p- dioxin, 2,3,7,8- (TCDD)	001746-01-6	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	0	0	6	0.0002	Yes	Yes
Tetrachlorodibenzofuran, 2,3,7,8-	051207-31-9	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	5000	5000	50000	50000	0	0	6	0.0002	Yes	Yes
Tetrachloroethane, 1,1,2,2-	000079-34-5	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	5	5	5	5	100	1000	11	1	Yes	No
Tetrachloroethylene	000127-18-4	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	500	50	500	100	1000	17	1	Yes	No
Tetrahydrothiophene, 1, 1-dioxide	000126-33-0	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	0.5	0.5	0.5	0.5	1	1	11	0.2	Yes	Yes
Thallium	007440-28-0	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	50	500	50	100	1000			No	Yes
Toluene	000108-88-3	10	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	5000	50	100	100	17	1	Yes	No
Toxaphene	008001-35-2	1000	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	50000	50000	50000	50000	10000	10000	6	0.002	Yes	Yes
Tributyltin	000688-73-3	10000	1.0E+00	1.0E-04	2.0E-05	2.0E-09	1	1	50000	50000	50000	50000	10000	10000	17	0.2	Yes	Yes
Tributyltin chloride	001461-22-9	10000	1.0E+00	1.0E-04	2.0E-01	2.0E-05	1	1	500	50000	50000	50000	10000	10000	17	0.2	Yes	Yes
Tributyltin oxide	000056-35-9	10000	1.0E+00	1.0E-04	2.0E-01	2.0E-05	1	1	500	50000	5000	50000	10000	10000	6	0.002	Yes	Yes
Trichlorobenzene, 1,2,4-	000120-82-1	1000	1.0E+00	1.0E-02	2.0E-01	2.0E-03	0.4	0.4	5000	500	5000	500	1000	10000	17	1	Yes	No

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			Ground Water Mobility			Persistence			Bioacc	cumulation		Facto	oxicity								
			L	iquid	Nor	n-Liquid	- reisi	stence	Food	Chain	Envir	onment	_ ECOIC	xicity	Air Gas	Air Gas					
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migration			Part			
Trichloroethane, 1,1,1-	000071-55-6	1	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	10	100	17	1	Yes	No			
Trichloroethane, 1,1,2-	000079-00-5	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	5	5	5	5	100	10	17	1	Yes	No			
Trichloroethylene	000079-01-6	1000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	100	10	17	1	Yes	No			
Trichlorofluoromethane	000075-69-4	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	1	50	50	50	50	0	0	17	1	Yes	No			
Trichlorophenol, 2,4,6-	000088-06-2	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	0.4	5000	5000	50000	50000	1000	100	11	0.2	Yes	Yes			
Trichlorophenoxyacetic acid, 2,4,5- (2,4,5-T)	000093-76-5	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	0.4	500	500	500	500	10000	100	6	0.02	Yes	Yes			
Trichloropropane, 1,2,3-	000096-18-4	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	50	50	10	10	11	1	Yes	No			
Trifluralin (Treflan)	001582-09-8	100	1.0E+00	1.0E-04	2.0E-03	2.0E-07	1	1	5000	5000	50000	50000	10000	10000	11	0.02	Yes	Yes			
Trinitrobenzene, 1,3,5-	000099-35-4	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	5	5	5	1000	1000	0	0.002	Yes	Yes			
Uranium	007440-61-1	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	1	1	0.5	0.5	0.5	0.5	100	100			No	Yes			
Vanadium	007440-62-2	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	500	50000	50000	100	100			No	Yes			
Vinyl Acetate	000108-05-4	10	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.4	0.4	0.5	0.5	0.5	0.5	10	100	17	1	Yes	No			
Vinyl Chloride	000075-01-4	10000	1.0E+00	1.0E+00	1.0E+00	1.0E+00	0.0007	0.07	5	5	5	5	0	0	17	1	Yes	No			
Xylene, P-	000106-42-3	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	50	50	100	100	17	1	Yes	No			
Xylene, m-	000108-38-3	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	500	500	500	500	100	100	17	1	Yes	No			
Xylene, o-	000095-47-6	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	50	50	100	100	17	1	Yes	No			
Xylenes	001330-20-7	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	0.4	1	50	50	50	50	100	100	17	1	Yes	No			
Zinc	007440-66-6	10	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	50000	50000	50000	10	100	•••		No	Yes			

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				Ground Wate	er Mobility	7	Dorai	stanaa		Bioacc	cumulation		Easts	oxicity				
			L	iquid	Nor	n-Liquid	Persi	stence	Food	Chain	Envir	onment	_ ECOU	oxicity	Air Gas Air Gas			
Substance Name	CAS Number	Toxicity	Karst	Non-Karst	Karst	Non-Karst	River	Lake	Fresh	Salt	Fresh	Salt	Fresh	Salt	Migration			Part
Americium 241(radionuclide)	014596-10-2	10000	1.0E+00	1.0E-02			1	1	0.5	0.5	0.5	0.5	10000	10000			No	Yes
Antimony 125(+D) (radionuclide)	014234-35-6	1000	1.0E+00	1.0E+00			1	1	0.5	0.5	0.5	0.5	1000	1000			No	Yes
Cadmium 109(radionuclide)	014109-32-1	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50000	50000	50000	50000	1000	1000			No	Yes
Cesium 137(+D) (radionuclide)	010045-97-3	10000	1.0E+00	1.0E+00			1	1	0.5	0.5	0.5	0.5	10000	10000			No	Yes
Cobalt 57(radionuclide)	013981-50-5	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50	5000	50	5000	100	100		•••	No	Yes
Cobalt 60(radionuclide)	010198-40-0	10000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	50	5000	50	5000	10000	10000			No	Yes
Iron 55(radionuclide)	014681-59-5	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5000	5000	50000	5000	100	100			No	Yes
Lead 210(+D) (radionuclide)	014255-04-0	10000	1.0E+00	1.0E+00			1	1	0.5	0.5	0.5	0.5	10000	10000			No	Yes
Manganese 54(radionuclide)	013966-31-9	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	500	50000	50000	50000	1000	1000			No	Yes
Nickel 59(radionuclide)	014336-70-0	100	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	5	50000	5	100	100			No	Yes
Nickel 63(radionuclide)	013981-37-8	1000	1.0E+00	1.0E-02	1.0E+00	1.0E-02	1	1	5	5	50000	5	1000	1000			No	Yes
Plutonium 236(radionuclide)	015411-92-4	10000	1.0E+00	1.0E+00	•••	•••	1	1	50	50	500	500	10000	10000	•••		No	Yes
Plutonium 238(radionuclide)	013981-16-3	10000	1.0E+00	1.0E+00		•••	1	1	50	50	500	500	10000	10000			No	Yes
Plutonium 239(radionuclide)	015117-48-3	10000	1.0E+00	1.0E+00		•••	1	1	50	50	500	500	10000	10000			No	Yes
Plutonium 240(radionuclide)	014119-33-6	10000	1.0E+00	1.0E+00		•••	1	1	50	50	500	500	10000	10000			No	Yes
Plutonium 241 (+D) (radionuclide)	014119-32-5	0	1.0E+00	1.0E+00		•••	1	1	0.5	0.5	0.5	0.5	0	0			No	Yes
Plutonium 242(radionuclide)	013982-10-0	10000	1.0E+00	1.0E+00		•••	1	1	50	50	500	500	10000	10000			No	Yes
Plutonium 243(radionuclide)	015706-37-3	100	1.0E+00	1.0E+00			0.07	0.07	50	50	500	500	100	100			No	Yes

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Uranium 232(radionuclide) 014158-29-3

10000

1.0E+00

1.0E+00

1.0E+00

1.0E+00

0.5

0.5

0.5

0.5

10000

10000

No Yes

Ground Water Mobility Bioaccumulation Persistence Ecotoxicity Liquid Non-Liquid Food Chain Environment Air Gas Air Gas MigrationMobility Gas Part Substance Name CAS Number Toxicity Non-Karst Lake Salt Karst Karst Non-Karst River Fresh Salt Fresh Salt Fresh Plutonium 244(+D) 014119-34-7 10000 1.0E+00 1.0E+00 1 0.5 0.5 0.5 0.5 10000 10000 No Yes (radionuclide) Radium 226(+D) 013982-63-3 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes (radionuclide) Radium 228(+D) 015262-20-1 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes (radionuclide) Radon 222(+D) 014859-67-7 1000 1.0E+000.4 0.5 0.5 0.5 0.5 1000 1000 Yes No (radionuclide) Silver 108m(+D) 0 0 014391-65-2 0 1.0E+00 1.0E+000.5 0.5 0.5 0.5 No Yes (radionuclide) Silver 110m(radionuclide) 014391-76-5 1000 1.0E+001.0E+00 1.0E+00 50 50000 50 50000 1000 1000 1.0E+00No Yes 010098-97-2 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 10000 10000 Yes Strontium 90(+D) 0.5 No (radionuclide) Technetium 014133-76-7 1000 1.0E+00 1.0E+000.5 0.5 0.5 0.5 1000 1000 No Yes 99(radionuclide) Thallium 204(radionuclide) 013968-51-9 1000 1.0E+001.0E-02 1.0E+00 1.0E-02 500 50 500 50 1000 1000 No Yes Thorium 227(radionuclide) 015623-47-9 10000 1.0E+00 1.0E-02 0.4 0.5 0.5 0.5 0.5 10000 10000 No Yes Thorium 228(+D) 014274-82-9 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes (radionuclide) 0.5 Thorium 229(+D) 015594-54-4 10000 1.0E+00 1.0E+000.5 0.5 0.5 10000 10000 No Yes (radionuclide) Thorium 230(radionuclide) 014269-63-7 10000 1.0E+00 1.0E-02 0.5 0.5 0.5 0.5 10000 10000 No Yes Thorium 231(radionuclide) 014932-40-2 1000 1.0E+00 1.0E-02 0.4 0.07 0.5 0.5 0.5 0.5 1000 1000 No Yes 0.5 Thorium 232(radionuclide) 007440-29-1 10000 1.0E+000.5 0.5 0.5 10000 10000 1.0E-02 No Yes Thorium 234(radionuclide) 015065-10-8 10000 1.0E+00 1.0E-02 0.5 0.5 0.5 0.5 10000 10000 No Yes Tritium(radionuclide) 010028-17-8 100 1.0E+00 1.0E+000.5 0.5 0.5 0.5 100 100 17 Yes No

(radionuclide)
Zinc 65(radionuclide)

013982-39-3

1000

1.0E+00

1.0E-02

1.0E+00

1.0E-02

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Publication Date: 06/20/2014

No Yes

Ground Water Mobility Bioaccumulation Persistence Ecotoxicity Liquid Food Chain Non-Liquid Environment Air Gas Air Gas MigrationMobility Gas Part Substance Name CAS Number Toxicity Karst Non-Karst Karst Non-Karst River Lake Fresh Salt Fresh Salt Salt Fresh Uranium 233(radionuclide) 013968-55-3 10000 1.0E+00 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes 1.0E+00 Uranium 234(radionuclide) 013966-29-5 10000 1.0E+00 1.0E+00 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes Uranium 235(+D) 015117-96-1 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 No Yes (radionuclide) Uranium 236(+D) 0 0.5 0 0 013982-70-2 1.0E+00 1.0E+00 0.5 0.5 0.5 No Yes (radionuclide) Uranium 238(+D) 10000 1.0E+00 1.0E+00 0.5 0.5 0.5 0.5 10000 10000 024678-82-8 No Yes

500

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